Instituto Nacional de Matemática Pura e Aplicada

Graph Continued Fractions

Thomás Jung Spier

Advisor: Carlos Gustavo Moreira
Co-advisor: Dimitar K. Dimitrov

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Contents

List of Symbols

$\mathcal{M}_G$ The set of all matchings of the graph G. 8

$\bar{c}_{T,j}$ The unique path from the root of the tree T to its vertex j. 37

∂S The frontier of the set S. 21

$\partial_i p$ The partial derivative with respect to x_i of the multivariate polynomial p. 5

$\phi(G)$ The multivariate characteristic polynomial of the weighted graph G. 3

ρ_c The weight of the directed cycle c. 4

ρ_c The weight of the path c when the edge weights are ρ_{ij}. 6

$adj(A_G(x))$ The adjugate of the matrix $A_G(x)$. 7

$c_{T,j}$ The unique path from the root of the tree T to its vertex j minus its last vertex j. 37

$def(G)$ The number of vertices left uncovered by a maximum matching in G. 21

$m_\theta(G)$ The multiplicity of θ as a zero of the matching polynomial of G. 24

p_n The number of self-avoiding walks of length n in a rooted locally-finite vertex-transitive graph. 77

t_c^m The sum of the weights of walks of length m from the root i to the last vertex of the path c in the path tree T_G^i. 19

t_i^m The sum of the weights of the closed tree-like walks of length m starting at vertex i. 18

z_G The largest zero of the matching polynomial of the weighted graph G. 34

$+_{\theta,G}$ The set of vertices of the weighted graph G such that their graph continued fractions are positive at θ. 25

$-_{\theta,G}$ The set of vertices of the weighted graph G such that their graph continued fractions are negative at θ. 25

$0_{\theta,G}$ The set of vertices of the weighted graph G such that their graph continued fractions are zero at θ. 25

$A_G(x)[i,j]$ The matrix obtained by deleting row i and column j from $A_G(x)$. 7

A_G The multivariate adjacency matrix of the weighted graph G. 3

C_G The set of vertices of the graph G that are neither essential nor have an essential vertex as neighbor. 21

$SubDisc_k(p)$ The k-subdiscriminant of the polynomial p. 64

$\alpha_i(G)$ The graph continued fraction of a weighted graph G with root i. 13

$\infty_{\theta,G}$ The set of vertices of the weighted graph G such that their graph continued fractions are infinite at θ. 25

$\lambda_{i\sim j}$ The contraction weight between the vertices i and j. 15

$\mu(G)$ The multivariate matching polynomial of the weighted graph G. 8

μ_G The connective constant of the locally-finite vertex-transitive graph G. 78

$\pm_{\theta,G}$ The set of vertices of the weighted graph G such that their graph continued fractions are positive or negative at θ. 25

Chapter 1

Introduction

This thesis focuses on a connection between matching polynomials and branched continued fractions.

The first known use of matching polynomials dates back to Riordan's work [94, p. 165], where he defined a variation for bipartite graphs known as rook polynomial and used it to study permutations with restrictions. At the beginning of the 70's, the matching polynomial appeared in the context of chemistry and physics. In chemical research, it appeared as a theoretical model of aromaticity and resonance energy in the works of Aihara, Gutman, Milun and Trinajstić [2, 60, 61]. In statistical physics, it appeared as the partition function of the monomer-dimer model in a classic paper by Heilmann and Lieb [64].

The matching polynomial was then studied from a mathematical perspective in a series of works by Farell, Godsil and Gutman [37, 55, 56], and is currently considered a relevant part of algebraic graph theory [52]. A comprehensive overview of the matching polynomial's early history is available in Gutman's survey [59].

In recent years, the matching polynomial has appeared in new contexts, such as: the construction of infinite bipartite ramanujan graphs for all degrees [85]; as an example in the theory of hyperbolic polynomials [3]; in a quantum computing framework known as gaussian boson sampling [20]; on an upper bound for the number of spanning forests of regular graphs [14].

We observe that the enumeration and search of matchings is a classic subject of combinatorics and complexity theory itself, as can be seen in Propp's survey [93] and Lovasz and Plummer's book [82].

On the other hand, there is the classic theory of continued fractions, which appears in connection with Pell's equation, orthogonal polynomials [69] and generating functions [44], to name a few. A good description of this theory is given in the books by Perron [89, 90], Jones and Thron [67] and Khrushchev [69].

In this thesis we are interested in a generalization of continued fractions, called branched continued fractions, that was introduced by Skorobogat'ko, Dronjuk, Bobik and Ptasnik [96]. There are several works that aim to generalize convergence theorems of continued fractions for this setting [17]. Recently, a more general type of branched continued fraction was also considered in two papers by Pétréolle, Sokal and Zhu [91, 92] that study some notions of positivity for combinatorial sequences of polynomials.

It turns out that there is a fundamental connection at a generating function level between matching polynomials and branched continued fractions that first appears in Viennot's work [101, p. 149]. In the same way that the characteristic polynomial of a graph is connected to determinants of symmetric matrices, the matching polynomial is related to branched continued fractions. In the first part of this thesis, we recall some basic facts about characteristic and matching polynomials and present this connection. From there, we develop our results.

On the matching polynomial side, in Chapter 3, we offer a conceptually simple proof of a Heilmann and Lieb theorem, which states that matching polynomials have real zeros. We then prove a refinement of a theorem by Ku and Wong [77], which extends the classic Gallai-Edmonds decomposition [35, 46] to the setting of weighted matching polynomials. A corollary of this theorem by Ku and Wong is a result by Ku and Chen [71], which states that the matching polynomials of vertex-transitive graphs have distinct zeros.

The main motivation for this theorem by Ku and Chen was presented in an article by Godsil [53]. As noted by Godsil, if a graph has a path of length l, then its matching polynomial has at least $l+1$ zeros. But there is a conjecture by Lovasz [81], which predicts that every vertex-transitive graph have Hamiltonian paths. Therefore, if this conjecture is true, then the matching polynomials of vertex-transitive graphs have distinct zeros, which is precisely what Ku and Chen proved.

Also for this reason, after proving the refined Gallai-Edmonds theorem for matching polynomials, we focus in Chapters 3 and 4 on better understanding the relationship between matching polynomials and paths in graphs. This theme is developed in three directions.

First, we prove a generalization for matching polynomials of a modification by Sylvester [98] of the classical Sturm's theorem [97] about the number of zeros of a real polynomial in an interval. Second, we characterize the number of distinct zeros of a matching polynomial in terms of the dimension of a vector space generated by the matching polynomials of a family of subgraphs. And finally, we present an upper bound for the number of paths that start at some vertex i of a graph G using only the matching polynomials of G and $G \setminus i$.

In the last chapter of the thesis, we shift the focus and consider classical periodic continued fractions. We prove some formulas for means of continued fractions and show how they help to illuminate the role of continued fractions in the classical theory of the Pell equation.

Chapter 2

Spectral Graph Theory

In this chapter, we recall some classical results of spectral graph theory. First, we define the multivariate characteristic polynomial of a graph and present some of its properties. We then show the corresponding results for the multivariate matching polynomial of a graph. Finally, we present the connection between multivariate matching polynomials and branched continued fractions.

2.1 Characteristic Polynomial

In this section, we present some properties of multivariate characteristic polynomials of graphs. All results from this section are obvious modifications from those presented in Godsil's book [52, p. 19, Chpt. 2–4].

Let G be a complete graph with vertex set $[n] := \{1, 2, \dots, n\}$. Define variable weights x_i and real weights ρ_{ij} for each of the vertices and edges, respectively. Considering edges with weight set to zero as non-existent, this definition captures all graphs. Two vertices i and j are *neighbors* if ρ_{ij} is non-zero. A graph defined in this way is a *weighted graph.*

The *multivariate adjacency matrix* of G is the symmetric matrix $A_G = (a_{i,j})_{i,j \in [n]}$ where $a_{i,j} = a_{j,i}$ is equal to ρ_{ij} if i is different from j, and $a_{i,i} = x_i$ for every i. The *multivariate characteristic polynomial* of G, denoted by $\phi(G)$, is defined as the determinant of A_G. This is a real multivariate polynomial on the n vertex variables x_i. It is also convenient to set $\phi(\emptyset) = 1$.

Two weighted graphs G and G' are *isomorphic* if there exists a bijection between their vertex sets that preserves edges and the vertex and edge weights. In general, if G and G' are isomorphic weighted graphs, then the multivariate adjacency matrices A_G and $A_{G'}$ are different. However, there will be an $n \times n$ permutation matrix P such that $PA_{G'}P^T = A_G$. This implies that $\phi(G')$ equals $\phi(G)$ so that the multivariate characteristic polynomial depends only on the weighted graph and is well defined.

The multivariate characteristic polynomial of G has a natural interpretation in terms of a weighted counting of directed cycles on the graph G. A *directed cycle c* on the graph G is a finite cyclic sequence of distinct vertices $i_0, i_1, \dots, i_k$ where k is a natural number, for every j in $[k]$ the vertex i_j is neighbor of i_{j-1}, and i_0 and

i_k are neighbors. The length of a directed cycle is defined as its total number of vertices. Note that the directed cycle c is equal to $i_m, \dots, i_k, i_0, i_1, \dots, i_{m-1}$ for every m in $[k]$, but different in general from its reverse $i_k, \dots, i_1, i_0$. In fact, a directed cycle is equal to its reverse if, and only if, it has length 2. The weight of directed cycle c, denoted by ρ_c, is defined as $(-1)^k \rho_{i_0 i_1} \rho_{i_1 i_2} \cdots \rho_{i_{k-1} i_k} \rho_{i_k i_0}$.

A *disjoint union of directed cycles* C on the graph G is a set of directed cycles on G such that none of its cycles share a common vertex. For simplicity, write $i \notin C$ if the vertex i is not in one of the directed cycles of C. Denote by $\mathcal{C}_G$ the set of all disjoint unions of directed cycles on the graph G.

In this case, there is the following well known interpretation for the multivariate characteristic polynomial.

Lemma 1 (Multivariate characteristic polynomial and disjoint union of directed cycles)**.** *The multivariate characteristic polynomial of G is equal to a weighted sum over all disjoint unions of directed cycles on G, i.e.,*

$$\phi(G) = \sum_{C \in \mathcal{C}_G} \prod_{i \notin C} x_i \prod_{c \in C} \rho_c.$$

Proof. The proof follows the same lines as the one presented in Godsil's book [52, p. 20, Lem. 1.3]. For any $n \times n$ matrix $B = (b_{i,j})$, there is the following classic formula for its determinant,

$$\det B = \sum_{\sigma \in S_n} sign(\sigma) \prod_{i \in [n]} b_{i,\sigma(i)},$$

where S_n is the set of permutations of $[n]$.

Recall that every permutation can be written as a unique product of disjoint cyclic permutations and the sign of the permutation is $(-1)^m$ where m is the number of its even length cycles. Denote by C_σ the set of cycles with length at least 2 of the permutation σ. Observe that an element of $[n]$ does not belong to a cycle in C_σ if, and only if, it is a fixed point of σ. Write $i \in c$ if i belongs to the cycle c and $i \notin C_\sigma$ if i is a fixed point of the permutation σ.

Putting it all together, we have,

$$\det B = \sum_{\sigma \in S_n} \prod_{i \notin C_\sigma} b_{i,i} \prod_{c \in C_\sigma} sign(c) \prod_{j \in c} b_{j,\sigma(j)}.$$

Now, consider B equal to the adjacency matrix A_G of the graph G. Note that for each permutation σ in S_n, a cycle c in C_σ corresponds to a finite cyclic sequence of distinct vertices of G. Observe that the expression $sign(c) \prod_{j \in c} a_{j,\sigma(j)}$ is different from zero if, and only if, c corresponds to a directed cycle on G, and in this case $sign(c) \prod_{j \in c} a_{j,\sigma(j)}$ is equal to ρ_c. It follows that the product $\prod_{c \in C_\sigma} sign(c) \prod_{j \in c} a_{j,\sigma(j)}$ is different from zero if, and only if, C_σ corresponds to a disjoint union of directed cycles C on G, and in this case $\prod_{c \in C_\sigma} sign(c) \prod_{j \in c} a_{j,\sigma(j)}$ is equal to $\prod_{c \in C} \rho_c$.

As a consequence,

$$\phi(G) = \det A_G = \sum_{\sigma \in S_n} \prod_{i \notin C_\sigma} a_{i,i} \prod_{c \in C_\sigma} sign(c) \prod_{j \in c} a_{j,\sigma(j)} = \sum_{C \in \mathcal{C}_G} \prod_{i \notin C} x_i \prod_{c \in C} \rho_c.$$

□

The *disjoint union* of the weighted graphs G and H is the weighted graph denoted by $G \sqcup H$, where the vertex and edges with their respective weights come from the disjoint union of the vertex and edge sets of the graphs G and H. For a multivariate polynomial $p(x_1, \ldots, x_n)$ we denote by $\partial_i p$ its partial derivative with respect to x_i.

The Lemma 1 is useful for interpreting and proving results on multivariate characteristic polynomials, as the next corollary shows.

Corollary 2. *Let G and H be weighted graphs and consider a vertex i in G. Then:*

a) $\phi(G \sqcup H) = \phi(G) \cdot \phi(H)$*;*

b) $\partial_i \phi(G) = \phi(G \setminus i)$*.*

Proof. *a*) By Lemma 1, the multivariate characteristic polynomial is a weighted count of disjoint unions of directed cycles. Since every disjoint union of directed cycles of $G \sqcup H$ is associated with a pair of disjoint unions of directed cycles of G and H, the result immediately follows.

Another way to prove this item is to observe that after a permutation of the vertices of $G \sqcup H$ its adjacency matrix can be considered equal to,

$$A_{G \sqcup H} = \begin{bmatrix} A_G & 0 \\ 0 & A_H \end{bmatrix}.$$

In this case, the determinant of $A_{G \sqcup H}$ is clearly the product of the determinants of A_G and A_H.

b) By Lemma 1 it follows that,

$$\partial_i \phi(G) = \sum_{i \notin C \in \mathcal{C}_G} \prod_{\substack{j \notin C \\ j \neq i}} x_j \prod_{c \in C} \rho_c = \phi(G \setminus i).$$

□

A *walk* w in the graph G is a finite sequence of vertices $i_0, i_1, \ldots, i_k$ where for every j in $[k]$ the vertex i_j is a neighbor, or equal to, the vertex i_{j-1}. The walk w is said to be from i_0 to i_k. A *closed walk* is a walk such that the first and last vertices are equal. The length of a walk is defined as its total number of vertices minus one. The weight of walk w is defined as $a_{i_0 i_1} a_{i_1 i_2} \cdots a_{i_{k-1} i_k}$.

With these definitions, the powers of the graph's adjacency matrix have a natural interpretation in terms of the weighted count of walks between pairs of vertices.

Lemma 3 (Powers of adjacency matrix and walks)**.** *Let G be a weighted graph with adjacency matrix A_G and consider two of its vertices i and j. Then the sum of the weights of all walks from i to j of length m is equal to $(A_G^m)_{i,j}$.*

Proof. For a proof see Godsil's book [52, p. 22, Lem. 2.1]. □

The multivariate characteristic polynomial also has a connection with paths on the graph, which are a special kind of walk. A *path* is a walk which does not repeat vertices. The weight of path c given by the sequence of vertices $i_0, i_1, \dots, i_k$ is $\rho_c := \rho_{i_0 i_1}\rho_{i_1 i_2}\cdots\rho_{i_{k-1}i_k}$. For two vertices i and j in the graph G denote by $[i \to j]$ the set of paths from i to j.

In this case, there is the following formula for the Wronskian of a multivariate characteristic polynomial.

Lemma 4. *For every two vertices i and j it holds,*

$$\partial_i\phi(G)\cdot\partial_j\phi(G) - \partial_i\partial_j\phi(G)\cdot\phi(G) = \phi(G\setminus i)\phi(G\setminus j) - \phi(G\setminus\{i,j\})\phi(G) =$$

$$= \left(\sum_{c\in[i\to j]}\rho_c\cdot\phi(G\setminus c)\right)^2.$$

Proof. For proof, see Godsil's book [52, p. 56, Cor. 2.2]. □

A *stable polynomial* is a polynomial p in $\mathbb{R}[x_1,\dots,x_n]$ such that whenever $\operatorname{Im} x_i > 0$ for every i in $[n]$, it holds that $p(x_1,\dots,x_n)\neq 0$. Using Lemma 4 it is possible to prove that the multivariate characteristic polynomial of a graph is stable.

Corollary 5. *For every weighted graph G its multivariate characteristic polynomial is stable.*

Proof. For proof of a generalization of this fact see Wagner's work [102, p. 71, Thm. 6.1]. □

These are all the results for multivariate characteristic polynomials that will be used in this work. From here on we focus on the special case where all vertex weights are a linear monic polynomial on the same variable. Given a graph G, the vertex weight of i is equal to $x_i = x - r_i$, where r_i is a real number. In this way, the adjacency matrix of G has the diagonal elements as linear monic polynomials in the same variable x. In this context, the weight of the walks is considered with respect to the adjacency matrix $A_G(0)$, as will become clear in the next results.

If the vertex weights are all equal to x and the edge weights are all equal to 1 then the multivariate characteristic polynomial of G is equal to the classical characteristic polynomial.

In this context, there is the classical Cauchy's interlace theorem, connecting the eigenvalues of a weighted graph with the those of its vertex deleted subgraphs. Recall that if polynomials $p(x)$ and $q(x)$ have all real zeros $r_1 \le r_2 \le \cdots \le r_n$ and $s_1 \le s_2 \le \cdots \le s_{n-1}$, respectively, then we say that p and q *interlace* if,

$$r_1 \le s_1 \le r_2 \le s_2 \le \cdots \le s_{n-1} \le r_n.$$

Corollary 6 (Cauchy's Interlacing theorem)**.** *For every weighted graph G, its characteristic polynomial $\phi(G)$ has real zeros. Furthermore, for every vertex i, the polynomials $\phi(G)$ and $\phi(G \setminus i)$ interlace.*

Proof. A short proof is available in Fisk's work [43, p. 1, Cor. 1]. $\square$

Of special interest for this work is the generating function for closed walks from a given vertex of a graph.

Lemma 7 (Generating functions for closed walks from a given vertex)**.** *Let i be a vertex in the graph G. Then the generating function for closed walks starting at i is,*

$$\sum_{m \geq 0} \frac{(-1)^m (A_G^m(0))_{i,i}}{x^{m+1}} = \frac{\phi(G \setminus i)}{\phi(G)}(x).$$

Proof. The proof is the same as in Godsil's book [52, p. 52, Lem. 1.1]. Consider the series,

$$\sum_{m \geq 0} \frac{(-1)^m A_G^m(0)}{x^{m+1}} = (x \cdot I_n + A_G(0))^{-1} = A_G(x)^{-1} = \frac{adj(A_G(x))}{\det A_G(x)} = \frac{adj(A_G(x))}{\phi(G)(x)},$$

where $adj(A_G(x))$ is the *adjugate* of the matrix $A_G(x)$.

Let $A_G(x)[i,j]$ denote the matrix obtained by deleting row i and column j from $A_G(x)$. Recall that, by definition, $(adj(A_G(x)))_{i,j}$ is $(-1)^{i+j} \det A_G(x)[i,j]$. This implies that,

$$\sum_{m \geq 0} \frac{(-1)^m (A_G^m(0))_{i,i}}{x^{m+1}} = \frac{(adj(A_G(x)))_{i,i}}{\phi(G)(x)} = \frac{(-1)^{2i} \det A_G(x)[i,i]}{\phi(G)(x)} = \frac{\phi(G \setminus i)}{\phi(G)}(x).$$

$\square$

The item (b) of Corollary 2 has the following immediate consequence which can be combined with the previous lemma.

Lemma 8 (Derivative of the characteristic polynomial)**.** *Let G be a weighted graph. Then,*

$$\phi(G)'(x) = \sum_{i \in [n]} \phi(G \setminus i)(x),$$

and, as a consequence,

$$\frac{\phi(G)'}{\phi(G)}(x) = \sum_{i \in [n]} \frac{\phi(G \setminus i)}{\phi(G)}(x).$$

As a corollary of Lemmas 7 and 8 the generating function for all closed walks in a graph has a neat expression in terms of the logarithmic derivative of its characteristic polynomial. This result is also present in Godsil's book [52, p. 23, Lem. 2.2].

Corollary 9 (Generating function for all closed walks)**.** *For every weighted graph G, the generating function for all of its closed walks is,*

$$\sum_{m\geq 0} \frac{(-1)^m}{x^{m+1}} \sum_{i\in[n]} (A_G^m(0))_{i,i} = \sum_{i\in[n]} \frac{\phi(G\setminus i)}{\phi(G)}(x) = \frac{\phi(G)'}{\phi(G)}(x).$$

There is also a formula due to Godsil [52, p. 53, Cor. 1.3] for the generating function of all walks between a fixed pair of distinct vertices.

Theorem 10 (Generating functions for walks between distinct vertices)**.** *Let i and j be different vertices in G. Then the generating function for walks starting at i and ending at j is,*

$$\sum_{m\geq 0} \frac{(-1)^m (A_G^m(0))_{i,j}}{x^{m+1}} = \frac{\sqrt{\phi(G\setminus i)\phi(G\setminus j) - \phi(G\setminus\{i,j\})\phi(G)}}{\phi(G)}(x) =$$

$$= \sum_{c\in[i\to j]} \frac{\rho_c \cdot \phi(G\setminus c)}{\phi(G)}(x).$$

Proof. For proof of first equality, see Godsil's book [52, p. 53, Cor. 1.3]. The second equality comes from Lemma 4. □

A *tree* is a graph for which there is exactly one path between each pair of distinct vertices, and a *forest* is a disjoint union of trees. Note that in the particular case of forests the last sum in Theorem 10 becomes simpler.

2.2 Matching Polynomial

In this section, following Godsil's book [52, p. 1, Chpt. 1], we present some properties of multivariate matching polynomials.

Let G be a weighted graph with vertex set $[n]$. Consider variable weights x_i and non-positive weights λ_{jk} for each of the vertices and edges, respectively. Considering edges with weight set to zero as non-existent, this definition captures all graphs. Two vertices i and j are neighbors if λ_{ij} is non-zero.

A *matching* in G is a set of edges, none of which have a vertex in common. Denote by $\mathcal{M}_G$ the set of all matchings of G. For simplicity write $i \notin M$ if the vertex i is not covered by the matching M, i.e., none of the edges of matching M are incident to i. Then the *multivariate matching polynomial* of G is defined as,

$$\mu(G) := \sum_{M\in\mathcal{M}_G} \prod_{i\notin M} x_i \prod_{jk\in M} \lambda_{jk}.$$

This is a real multivariate polynomial in the n vertex variables x_i. It is also convenient to define $\mu(\emptyset) = 1$. In Figure 2.1 we present an example of a weighted graph and its multivariate matching polynomial.

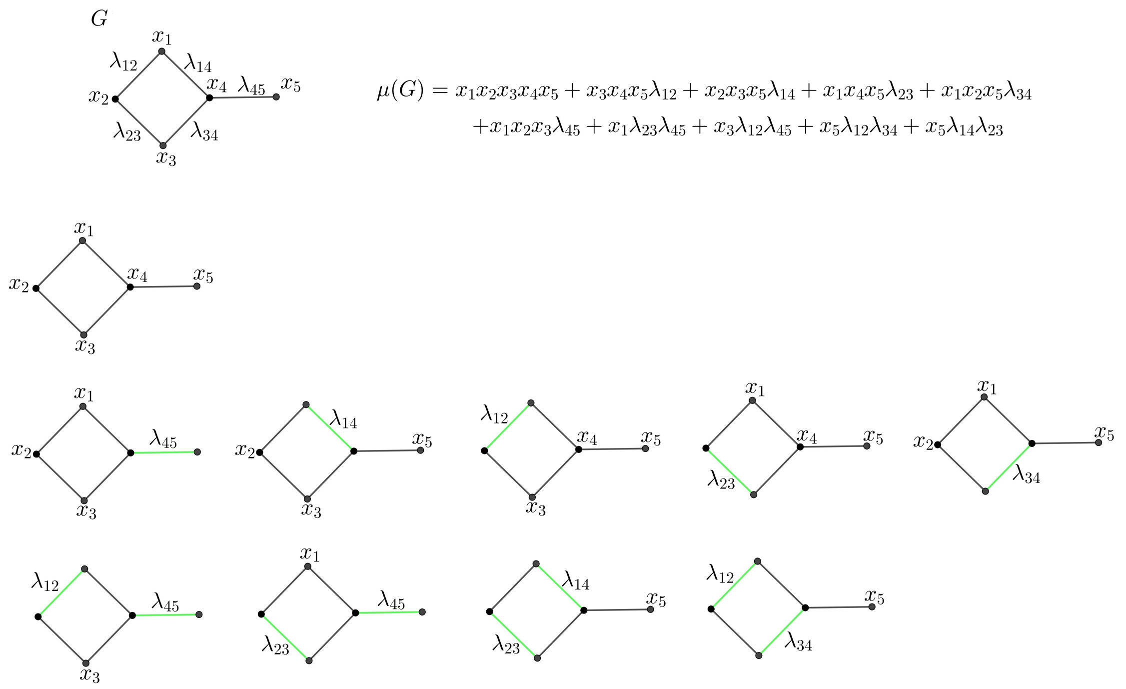


Figure 2.1: In this figure, G is a weighted graph and $\mu(G)$ is its multivariate matching polynomial. In the second, third and fourth lines are presented the matchings of G with 0, 1 and 2 edges, respectively, with their respective weights.

For a given graph, if all vertex weights are equal to x and all the edge weights are -1 then its multivariate matching polynomial is equal to its classical matching polynomial. The classical matching polynomial evaluated at $\sqrt{-1}$ gives the total number of matchings in the graph up to a power of $\sqrt{-1}$. A *perfect matching* is a matching that leaves no vertices uncovered. The constant coefficient of the classical matching polynomial gives the total number of perfect matchings in the graph up to a sign.

The multivariate matching polynomial satisfies a number of recurrences. The next lemma, which appears in Godsil's book [52, p. 2, Thm. 1.1], presents these recurrences and should be compared to Lemma 2.

Lemma 11. *Let G and H be weighted graphs and i and j be vertices in G. Then,*

a) $\mu(G \sqcup H) = \mu(G) \cdot \mu(H)$;

b) $\mu(G) = x_i\mu(G \setminus i) + \sum_{k \neq i} \lambda_{ik}\mu(G \setminus \{i,k\})$;

c) $\mu(G) = \lambda_{ij}\mu(G \setminus \{i,j\}) + \mu(G \setminus ij)$;

d) $\partial_i\mu(G) = \mu(G \setminus i)$.

Proof. *a*) Since the matchings of $G \sqcup H$ are a pair of matchings in G and H, the result follows.

b) The matchings of G that do not cover the vertex i contribute $x_i\mu(G \setminus i)$ to $\mu(G)$. The matchings of G which cover the vertex i must use one of the incident edges and therefore contribute $\sum_{k\neq i} \lambda_{ik}\mu(G \setminus \{i,k\})$ in total to $\mu(G)$.

c) If we separate the matchings of G into those that contain the edge ij, or not, the conclusion follows.

d) This item is an immediate consequence of item (*b*). □

Observe that the definition of the multivariate matching polynomial is reminiscent of Lemma 1. Given a weighted graph G, consider a new weighted graph $\hat{G}$ obtained from G where the new edge weights are $\rho_{ij} = \sqrt{-\lambda_{ij}}$. As in the previous section denote by ρ_c the weight of cycle c. Write $\mathcal{C}_{\hat{G},2}$ for the set of all disjoint unions of directed cycles with length two on the graph $\hat{G}$. In this case, there is the following interpretation for the multivariate matching polynomial.

Lemma 12 (Multivariate matching polynomial and disjoint union of directed cycles with length 2)**.** *The multivariate matching polynomial of G is equal to the weighted sum over all disjoint unions of directed cycles with length two on $\hat{G}$, i.e.,*

$$\mu(G) = \sum_{C \in \mathcal{C}_{\hat{G},2}} \prod_{i \notin C} x_i \prod_{c \in C} \rho_C.$$

Note that in Lemma 1 the counting is over all disjoint union of directed cycles rather than just those with length 2. In other words, the sum in Lemma 12 is over the set $\mathcal{C}_{\hat{G},2}$ which is a subset of $\mathcal{C}_{\hat{G}}$. The graphs for which the only directed cycles are those with length two are precisely forests. As a consequence, we have the following corollary that appears in Godsil's book [52, p. 21, Cor. 1.4].

Corollary 13. *The multivariate matching polynomial of G coincides with the multivariate characteristic polynomial of $\hat{G}$ if, and only if, G is a forest.*

Proof. Observe that $\phi(\hat{G}) - \mu(G) = \sum_{C \in \mathcal{C}_{\hat{G}} \setminus \mathcal{C}_{\hat{G},2}} \prod_{i \notin C} x_i \prod_{c \in C} \rho_C$. If G is a forest, then this last sum is clearly zero, which implies that the characteristic and matching polynomials coincide.

Now, let n be the number of vertices of $\hat{G}$ and g be the *girth* of $\hat{G}$, i.e., the length of the shortest cycle of $\hat{G}$. If G is not a forest, then g is bigger than, or equal to, 3. This, in turn, implies that there exists a term of degree $n-g$ in $\sum_{C \in \mathcal{C}_{\hat{G}} \setminus \mathcal{C}_{\hat{G},2}} \prod_{i \notin C} x_i \prod_{c \in C} \rho_C$ which is nonzero and therefore the characteristic and matching polynomials do not coincide. □

In particular, for a graph G, its classical matching polynomial is equal to its classical characteristic polynomial if, and only if, G is a forest. This result goes back at least to the work of Godsil and Gutman [56, p. 141, Cor. 4.2].

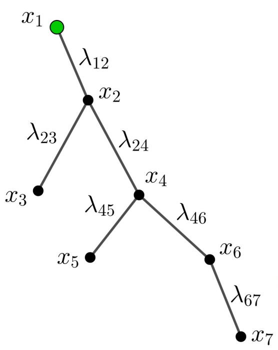
The statement of Corollary 13 motivates the following assumption that we will assume from now on. Given a weighted graph G, to compute its characteristic polynomial the edge weights are always assumed to be the negative of the square root of the edge weights used to compute its matching polynomial. With this assumption, the multivariate matching and characteristic polynomials of a forest always coincide.

2.3 Graph Continued Fractions

The multivariate characteristic polynomial is, by definition, connected to determinants of symmetric matrices. In this section, following Viennot's work [101, p. 149], we establish the connection between multivariate matching polynomials and branched continued fractions.

A *branched continued fraction* is a generalization of the classical continued fractions that was introduced in the work of Skorobogat'ko, Dronjuk, Bobik and Ptasnik [96]. There are several works that aim to generalize convergence theorems for branched continued fractions. For example, Bodnar, Voznyak and Mykhal'chuk [17, p. 70] claim that branched continued fractions with integer entries converge.

For every rooted weighted tree, a branched continued fraction can be associated in a natural way, as exemplified in Figure 2.2. We call a branched continued fraction obtained this way *tree continued fraction.*



$$\rightleftarrows \qquad x_1 + \cfrac{\lambda_{12}}{x_2 + \cfrac{\lambda_{23}}{x_3} + \cfrac{\lambda_{24}}{x_4 + \cfrac{\lambda_{45}}{x_5} + \cfrac{\lambda_{46}}{x_6 + \cfrac{\lambda_{67}}{x_7}}}}$$

Figure 2.2: A rooted weighted tree and its associated tree continued fraction.

In this case, the following result holds.

Theorem 14. *For a weighted tree T with root i, its associated tree continued fraction is equal to* $\dfrac{\mu(T)}{\mu(T \setminus i)}$.

Proof. For every graph G and vertex i, by item (b) of Lemma 11, it follows that,

$$\mu(G) = \sum_{j \neq i} \lambda_{ij} \mu(G \setminus \{i, j\}) + x_i \mu(G \setminus i) \iff \frac{\mu(G)}{\mu(G \setminus i)} = x_i + \sum_{j \neq i} \frac{\lambda_{ij}}{\dfrac{\mu(G \setminus i)}{\mu(G \setminus \{i, j\})}}.$$

To finish the proof, we replace the graph G for the tree T in this last equation and iterate the recurrence. $\square$

Looking at the proof of Theorem 14, it can be seen that, in principle, it should work more generally for every rooted graph, the only missing ingredient being the analogue of a tree continued fraction. When iterating the recurrence for a rooted graph the end result is a tree continued fraction for the rooted path tree of the rooted graph.

For a graph G with root i its *rooted path tree* T_G^i is the rooted tree with vertices labeled by paths in G starting at i. Two vertices are connected if one path is a maximal sub-path of the other. The root of T_G^i is the trivial path i, and the weights of T_G^i are taken from the weights of G, as exemplified in Figure 2.3.

This motivates the following definition.

Definition 15 (Graph continued fraction). *The graph continued fraction of a weighted graph G with root i is defined as* $\alpha_i(G) := \dfrac{\mu(G)}{\mu(G \setminus i)}$.

Note that this is consistent with the definition of tree continued fraction. The above observation leads to the following lemma, originally due to Godsil [50, p. 287, Thm. 2.5].

Lemma 16 (Godsil). *Let G be a weighted graph with root i. Then,*

$$\frac{\mu(G)}{\mu(G \setminus i)} = \alpha_i(G) = \alpha_i(T_G^i) = \frac{\mu(T_G^i)}{\mu(T_G^i \setminus i)}.$$

As a consequence of this lemma, every graph continued fraction can be transformed into a tree continued fraction. This also allows the definition of graph continued fractions for infinite graphs, which appears in Section 4.3.3. An illustration of the Lemma 16 is presented in Figure 2.3, where, for simplicity, the rooted graphs represent their graph continued fractions.

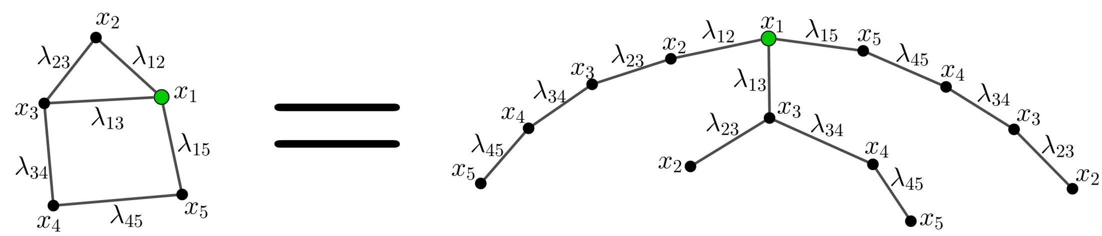


Figure 2.3: An illustration of the equality $\alpha_i(G) = \alpha_i(T_G^i)$ from the Lemma 16.

Using the Lemma 16 we can give a proof of the classic result of Heilmann and Lieb [64, p. 201-203, Thms. 4.3 and 4.6] about the position of the zeros of multivariate matching polynomials.

Theorem 17 (Heilmann-Lieb [64]). *The multivariate matching polynomial of G is nonzero if one of the following conditions is satisfied:*

- $\mathrm{Im}(x_i) > 0$ *for every i;*
- $|x_i| > 2\sqrt{B_G}$ *for every i, where B_G is equal to* $\max_j \max_{\substack{A \subseteq [n] \setminus j \\ |A| = n-2}} \sum_{k \in A} -\lambda_{jk}$ *if $n \geq 3$, and equal to $-\lambda_{12}/4$ or 0 if n is two or one, respectively.*

Proof. The approach is the same as in [64, p. 201-203, Thms. 4.3 and 4.6]. Consider a graph G and let R be the union of the regions $[\mathrm{Im}(x) > 0]$ and $[|x| > 2\sqrt{B_G}]$ in the complex plane. Our aim is to prove that $\mu(G)$ is different from zero in R^n. Note that for a graph with only one vertex this result is trivial. Assume, by induction hypothesis, that the statement is true for any graph with fewer vertices than G.

Choose any vertex i as a root of G. By the induction hypothesis, and $B_G \geq B_{G\setminus i}$, it suffices to prove that the graph continued fraction $\alpha_i(G) = \dfrac{\mu(G)}{\mu(G\setminus i)}$ is nonzero in R^n.

By Lemma 16, $\alpha_i(G)$ is equal to the tree continued fraction $\alpha_i(T_G^i)$. Following the rooted tree T_G^i structure, one can write $\alpha_i(G) = \alpha_i(T_G^i)$ as a composition of some of the functions,

$$f_{j,A}(x_1, \ldots, x_n) := x_j + \sum_{k\in A} \frac{\lambda_{jk}}{x_k},$$

with j in $[n]$ and A a subset of $[n] \setminus j$. Each function in the composition corresponds to a vertex in the rooted tree T_G^i. Observe that except for the last function in this composition, which corresponds to the root of T_G^i, all other functions $f_{j,A}$ satisfy $|A| \leq n-2$. This can be seen by carefully examining the examples in Figures 2.2 and 2.3.

Finally, notice that the image of R^n for each function $f_{j,A}$ with $|A| \leq n-2$ is again contained in R, and that each function $f_{j,A}$ with $|A| = n-1$ is nonzero in R^n. Putting all this together, it follows that $\alpha_i(G) = \alpha_i(T_G^i)$ is nonzero in R^n, which ends the proof. □

Although the proof of Theorem 17 is the original one, the interpretation in terms of composition of branched continued fractions seems to be new.

With the concept of graph continued fraction already in place, a natural question is the effect of graph operations on a graph continued fraction. We consider one of the simplest graph operations that exists, to remove a vertex from the graph. Notice that,

$$\alpha_i(G) - \alpha_i(G\setminus j) = \frac{\mu(G)}{\mu(G\setminus i)} - \frac{\mu(G\setminus j)}{\mu(G\setminus \{j,i\})} =$$
$$= \frac{\mu(G\setminus\{i,j\})\mu(G) - \mu(G\setminus i)\mu(G\setminus j)}{\mu(G\setminus\{i,j\})\mu(G\setminus i)}.$$

Thus, we are led to consider the expression $\mu(G\setminus i)\mu(G\setminus j) - \mu(G\setminus\{i,j\})\mu(G)$. The next lemma, which originally appears in the work of Heilmann and Lieb [64, p.213, Thm. 6.3], simplifies this last expression and is one of the main tools in the study of matching polynomials.

Lemma 18 (Christoffel-Darboux [64]). *Consider a graph G and two distinct vertices i and j. Then,*

$$\partial_i\mu(G)\cdot\partial_j\mu(G) - \partial_i\partial_j\mu(G)\cdot\mu(G) = \mu(G\setminus i)\mu(G\setminus j) - \mu(G\setminus\{i,j\})\mu(G) =$$

$$= \sum_{c \in [i \to j]} \lambda_c \cdot \mu(G \setminus c)^2,$$

where λ_c is the product of $-\lambda_e$ over the edges e of the path c.

Proof. Proof by induction on the number of vertices of the graph, as in the work of Heilmann and Lieb [64, p.213, Thm. 6.3]. □

Note that since the edge weights are non-positive, $-\lambda_c$ is non-positive for every path c. The Lemma 18 should also be compared to Lemma 4. There are also generalizations of both the Lemmas 4 and 18 in Gutman's work [58, p. 58].

Using Lemma 18 we also get a simplified formula for the effect of removing a vertex on a graph continued fraction,

$$\alpha_i(G) - \alpha_i(G \setminus j) = \frac{-\sum_{c \in [i \to j]} \lambda_c \cdot \mu(G \setminus c)^2}{\mu(G \setminus \{i,j\})\mu(G \setminus j)}.$$

This generalizes the classical continued fraction difference formula,

$$\frac{p_n}{q_n} := a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\ddots + \cfrac{1}{a_n}}}}, \ \forall n \in \mathbb{N} \implies \frac{p_n}{q_n} - \frac{p_{n-1}}{q_{n-1}} = \frac{(-1)^{n+1}}{q_{n-1}q_n}.$$

It turns out that it is useful to rewrite the difference formula for the graph continued fractions as follows.

Lemma 19 (Contraction)**.** *Let i and j be distinct vertices in the graph G. Then,*

$$\alpha_i(G) = \alpha_i(G \setminus j) + \frac{\lambda_{i\sim j}}{\alpha_j(G \setminus i)}, \ \textit{where } \lambda_{i\sim j} = \lambda_{j\sim i} := -\sum_{c \in [i \to j]} \lambda_c \cdot \left(\frac{\mu(G \setminus c)}{\mu(G \setminus \{i,j\})}\right)^2$$

is the contraction weight between the vertices i and j.

Since all the edges have non-positive weights, it follows that $-\lambda_{i\sim j}$ is a sum of squares. Furthermore, $\lambda_{i\sim j}$ does not depend on the vertex weights of i and j.

The Lemma 19 is our main lemma and will be very important in Section 3.1. It is well known in the classical theory of continued fractions, as can be seen in the books by Perron [90, p. 12, Satz 1.6] and Jones and Thron [67, p. 38]. Using Viennot's beautiful Heaps of Pieces theory [101, p. 149-150] it is also possible to give a combinatorial interpretation to Lemma 19 which clarifies the role of $\lambda_{i\sim j}$.

The next example shows one of the most used instances of the classic contraction lemma for continued fractions, as seen in Jones and Thron's book [67, p.42, Thm. 2.10].

Example 20 (Classic contraction lemma)**.** *The following equalities are true,*

$$1-\cfrac{\alpha_1}{1-\cfrac{\alpha_2}{1-\cfrac{\alpha_3}{1-\cfrac{\alpha_4}{1-\cfrac{\alpha_5}{1-\cdots}}}}}=1-\cfrac{\alpha_1}{1-\alpha_2-\cfrac{\alpha_2\alpha_3}{1-(\alpha_3+\alpha_4)-\cfrac{\alpha_4\alpha_5}{1-\cdots}}}=$$

$$=1-\alpha_1-\cfrac{\alpha_1\alpha_2}{1-(\alpha_2+\alpha_3)-\cfrac{\alpha_3\alpha_4}{1-(\alpha_4+\alpha_5)-\cfrac{\alpha_5\alpha_6}{1-\cdots}}}.$$

In Figure 2.4 it is shown how to represent the first continued fraction as a rooted graph and how to apply the Contraction Lemma 19 to prove the two equalities.

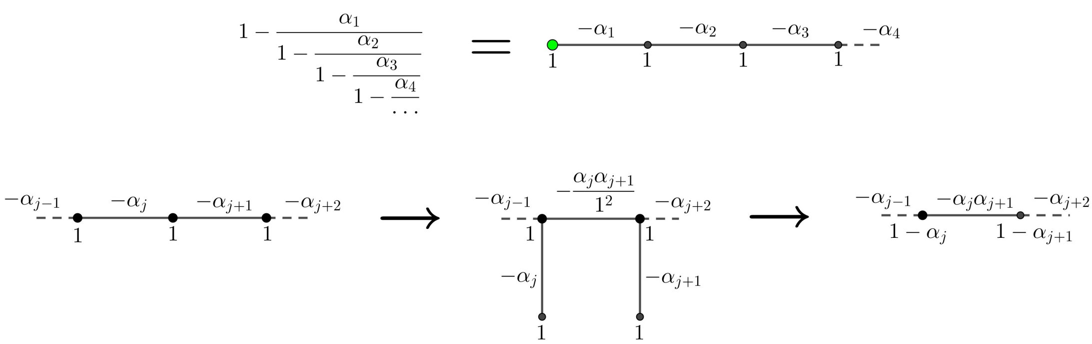


Figure 2.4: The first equality shows the representation of the continued fraction of Example 20 as a rooted graph. The second part shows how the Contraction Lemma 19 can be applied to prove the equalities of Example 20. Applying the the Contraction Lemma 19 with i and j equal to the $2k$-th and $(2k+2)$-th vertex of the graph continued fraction, respectively, for every natural number k, we obtain the first equality of Example 20. On the other hand, applying the the Contraction Lemma 19 with i and j equal to the $(2k-1)$-th and $(2k+1)$-th vertex of the graph continued fraction, respectively, for every natural number k, we obtain the second equality of Example 20.

The Contraction Lemma 19 also implies a simple formula for the derivative of a graph continued fraction.

Corollary 21. *Let i and j two distinct vertices of a graph G. Then,*

$$\partial_j\alpha_i(G)=\frac{-\lambda_{i\sim j}}{\alpha_j(G\setminus i)^2}.$$

Proof. This follows immediately from Lemma 19, because both $\alpha_i(G\setminus j)$ and $\lambda_{i\sim j}$ do not depend on x_j and $\partial_j\alpha_j(G\setminus i)=1$. □

For our next result we define the *rooted product of graphs*, which was originally introduced by Godsil and McKay [57, p. 21, Def'n 1.1].

Definition 22 (Rooted product of graphs [57])**.** *Let G be a graph in $[n]$ and H be a sequence of n rooted graphs $H_1, \ldots, H_n$. Then the rooted product of G by H, denoted by $G \circ H$, is the graph obtained by identifying the root of H_i with the i-th vertex of G.*

If G and $H_1, \ldots, H_n$ are weighted graphs, then weights can be assigned to $G \circ H$ in a natural way. For the vertex of $G \circ H$ which is the i-th vertex of G identified with the root of H_i assign the weight of the i-th vertex of G if H_i is empty or assign the weight of the root of H_i otherwise. The remaining vertices and edges of $G \circ H$ receive the weights in the obvious way.

In the particular case where all the rooted graphs of the sequence are equal to a same graph H with root j, we denote the rooted product of G by this special sequence as $G \circ_j H$.

The rooted product of graphs arises naturally in the composition of two graph continued fractions, as stated in the next lemma. This lemma and its connection to branched continued fractions seem to be new.

Lemma 23. *(Composition of graph continued fractions) Let G be a rooted graph in $[n]$ with root i, and consider a sequence H of rooted graphs $H_1, \ldots, H_n$ with roots $k_1, \ldots, k_n$, respectively. If x_j is set equal to $\alpha_{k_j}(H_j)$ for every j such that H_j is non-empty in $\alpha_i(G)(x_1, \ldots, x_n)$, then the result is equal to $\alpha_i(G \circ H)$.*

Proof. By Lemma 16 the graph continued fractions $\alpha_i(G)(x_1, \ldots, x_n)$, $\alpha_i(G \circ H)$ and $\alpha_{k_j}(H_j)$ for every j such that H_j is non-empty, are equal to the tree continued fractions of their respective path trees. Note that if we replace in the tree continued fraction of $\alpha_i(G)(x_1, \ldots, x_n)$ all variables x_j, for each j such that H_j is non-empty, by the tree continued fraction of $\alpha_{k_j}(H_j)$ we will obtain precisely the tree continued fraction of $\alpha_i(G \circ H)$. This proves the equality of the statement. $\square$

In the work [57, p. 22, Thm. 2.1] the authors also showed how the classical characteristic polynomials of a rooted product of graphs can be obtained from the respective polynomials of the graphs in the product.

The Lemma 23 is actually being used in the proof of the Theorem 17. Combining the Contraction Lemma 19, Godsil's Lemma 16 and Lemma 23 we can also give a simple proof of a formula for periodic continued fractions. This is shown in Figure 2.5. The proof of the formula in Figure 2.5 seems to be new. The formula shown in Figure 2.5 can be used as the starting point for *Pell's equation theory* [69, p. 84-92] in terms of continued fractions.

These are all the results for multivariate graph continued fractions that interest us. For the next result we focus in the special case where all the vertex weights are a linear polynomial in the same variable. Given a graph G the weight of the vertex i is assumed to be equal to $x_i = x - r_i$, where r_i is a real number for every i.

Of special interest in this case are the walks in the path tree T_G^i that start at the root. If i is a vertex in the graph G then these are called the *tree-like walks* starting

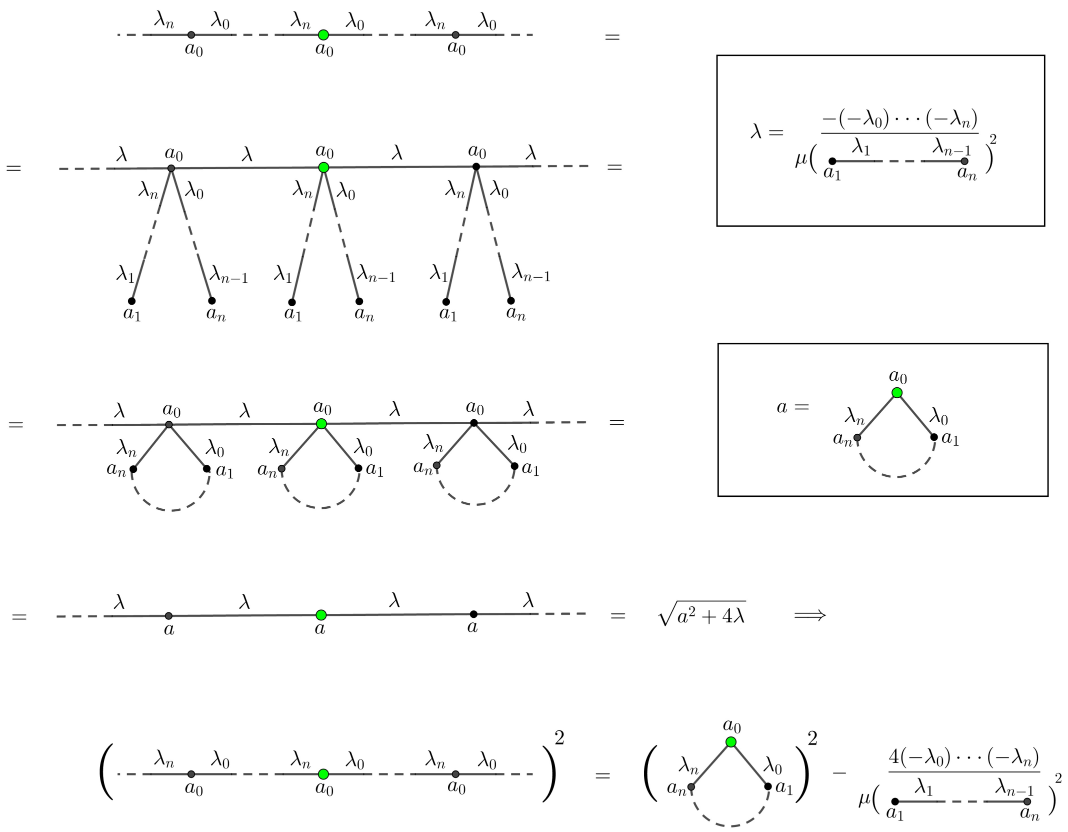


Figure 2.5: Formula for a periodic continued fraction. The first equality uses the Contraction Lemma 19, the second the Godsil's Lemma 16 and the third the Lemma 23. The fourth equality is a simple calculation.

at i. Denote by t_i^m the sum of the weights of all closed tree-like walks starting at i of length m. We are interested in the generating function for the sequence $(t_i^m)_{m\geq 0}$.

This generating function first appeared in an article by Godsil [50, p.292, Thm. 3.6]. The corresponding result when the graph is a path, but in terms of classical continued fractions and dyck paths, came a year earlier in Flajolet's work [44, p.129, Thm. 1]. An interpretation for graphs in terms of continued fractions appeared in Viennot's work [101, p. 149]. The next lemma, which appears in Godsil's work [50, p. 292, Thm. 3.6 (a)], presents the generating function for tree-like walks and should be compared to Lemma 7.

Lemma 24 (Generating function for closed tree-like walks [50])**.** *Let i be a vertex in G, then the generating function for the closed tree-like walks starting at i is,*

$$\sum_{m\geq 0} \frac{(-1)^m t_i^m}{x^{m+1}} = \frac{1}{\alpha_i(G)(x)}.$$

Proof. Observe that,

$$\sum_{m\geq 0}\frac{(-1)^m t_i^m}{x^{m+1}} = \frac{\phi(T_G^i\setminus i)}{\phi(T_G^i)}(x) = \frac{\mu(T_G^i\setminus i)}{\mu(T_G^i)}(x) = \frac{\mu(G\setminus i)}{\mu(G)}(x) = \frac{1}{\alpha_i(G)(x)}.$$

The first equality comes from Lemma 7, which gives the generating functions for closed walks starting at any vertex in any graph. Since T_G^i and $T_G^i \setminus i$ are trees the Corollary 13 implies that their matching and characteristic polynomials coincide, which gives second equality. The third and fourth equalities are simply the statement of Godsil's Lemma 16. □

Note that the item (d) of Lemma 11 has the following consequence which is known from the beginning of the matching polynomial history, as seen in Gutman's survey [59, p. 83, Thm. 5.3.6].

Lemma 25 (Derivative of the matching polynomial [59])**.** *For every weighted graph G, it holds,*

$$\mu(G)'(x) = \sum_{i\in[n]}\mu(G\setminus i)(x),$$

and, as a consequence,

$$\frac{\mu(G)'}{\mu(G)}(x) = \sum_{i\in[n]}\frac{\mu(G\setminus i)}{\mu(G)}(x).$$

Using the Lemmas 24 and 25 there is the following analogous statement of Corollary 9 which provides an expression for the generating function for all closed tree-like walks of a graph in terms of the logarithmic derivative of the matching polynomial. The next result appears in Godsil's work [50, p. 292, Thm. 3.6 (b)].

Corollary 26 (Generating function for all closed tree-like walks [50])**.** *For every graph G the generating function for all of its closed tree-like walks is,*

$$\sum_{m\geq 0}\frac{(-1)^m}{x^{m+1}}\sum_{i\in[n]}t_i^m = \sum_{i\in[n]}\frac{\mu(G\setminus i)}{\mu(G)}(x) = \frac{\mu(G)'}{\mu(G)}(x).$$

There is also an analogous version of Theorem 10 for tree-like walks.

Let $c : i \to j$ be a path in the graph G. Then c determines both a path and its final vertex in the path tree T_G^i. Denote by t_c^m the sum of the weights of walks of length m from the root i to the last vertex of the path c in the path tree T_G^i. Then there is the following formula for the generating series of $(t_c^m)_{m\geq 0}$ in terms of matching polynomials. The next result, although not stated in the literature, can be easily deduced from the results presented in Godsil's book [52] and is certainly well known.

Lemma 27 (Generating function for tree-like walks between different vertices [52])**.** *Let $c : i \to j$ be a path in the graph G. Then,*

$$\sum_{m\geq 0}\frac{(-1)^m t_c^m}{x^{m+1}} = \sqrt{\lambda_c}\frac{\mu(G\setminus c)}{\mu(G)}(x).$$

Proof. The proof is the same as in Lemma 24 with some minor observations. Note that,

$$\sum_{m\geq 0} \frac{(-1)^m t_c^m}{x^{m+1}} = \rho_c \frac{\phi(T_G^i \setminus c)}{\phi(T_G^i)}(x) = \sqrt{\lambda_c}\frac{\mu(T_G^i \setminus c)}{\mu(T_G^i)}(x) = \sqrt{\lambda_c}\frac{\mu(G \setminus c)}{\mu(G)}(x).$$

The first equality comes from Theorem 10, and notice that there is only one term instead of a sum because T_G^i is a tree. Recall that $\rho_{kl} = \sqrt{-\lambda_{kl}}$ for every two vertices k and l. This implies that $\rho_c = \sqrt{\lambda_c}$. Finally, one can give a simple proof by induction using Godsil's Lemma 16 that,

$$\frac{\mu(T_G^i \setminus c)}{\mu(T_G^i)}(x) = \frac{\mu(G \setminus c)}{\mu(G)}(x).$$

□

Chapter 3

Weighted Matching Polynomials

In the first section of this chapter, we present the classical Gallai-Edmonds Structure Theorem [35, 46] and prove a refined version of this theorem for graph continued fractions. In Section 3.2 we prove some easy lower bounds for the largest zero of a matching polynomial. In Section 3.3 we prove a generalization for matching polynomials of a modification by Sylvester [98] of the classical Sturm's theorem [97] about the number of zeros of a real polynomial in an interval. This generalization uses trees obtained as output of the depth first-search algorithm. Finally, in Section 3.4, we study the number of zeros of a matching polynomial in terms of the Gallai-Edmonds structure theorem for graph continued fractions.

3.1 Gallai-Edmonds Structure Theorem

Let G be a finite simple graph. The celebrated Gallai-Edmonds theorem [35, 46] gives the structure of maximum matchings in a graph. A *maximum matching* is a matching that uses as many edges as possible. An explanation of the Gallai-Edmonds decomposition and its consequences is present in the work of Lovász and Plummer [82, p. 94, Thm. 3.2.1].

A vertex v is covered by the matching M if there is an edge in M which is incident to v. The vertex v is *essential* if there is a maximum size matching in G which leaves v uncovered. If all the vertices of a graph are essential then the graph is called *factor-critical*. In this context, there is the following result by Gallai [46].

Theorem A (Gallai's lemma [46]). *If G is connected and factor-critical then each maximum matching leaves exactly one vertex uncovered.*

In particular, for each vertex of a connected factor-critical graph, there is a maximum matching that just leaves that vertex uncovered.

The *frontier* of a subset of vertices S of $[n]$ is defined as the set of vertices that are not in S but have a neighbor in S. The frontier of S is denoted by ∂S. Denote by D_G the set of essential vertices of G and define $C_G := [n] \setminus (D_G \cup \partial D_G)$. Denote by $def(G)$ the *deficiency* of G, i.e., the number of vertices left uncovered by a maximum matching in G.

Theorem B (Gallai-Edmonds structure theorem [35, 46])**.** *For every graph G it holds:*

a) The components of the subgraph induced by D_G are factor-critical;

b) The subgraph induced by C_G has a perfect matching;

c) Let S be a subset of ∂D_G. Then there are at least $|S|+1$ components of D_G which are connected to a vertex in S in the graph G;

d) If M is any maximum matching of G, it contains a matching that leaves exactly one vertex uncovered of each component of D_G, a perfect matching of each component of C_G and matches all points of ∂D_G with points in distinct components of D_G;

e) $def(G) = c(D_G) - |\partial D_G|$, where $c(D_G)$ denotes the number of connected components of the graph spanned by D_G.

In figure 3.1 we show an example of the Gallai-Edmonds decomposition for a graph.

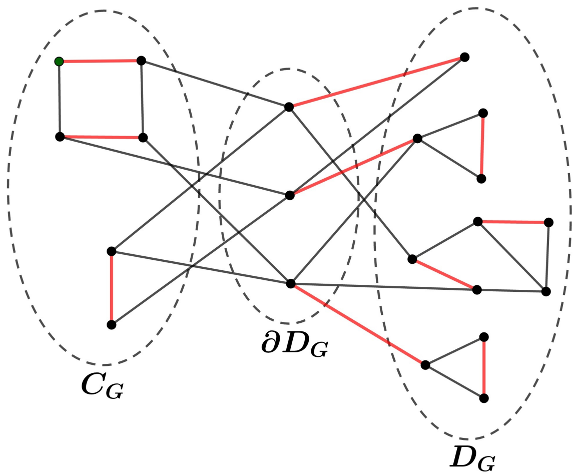


Figure 3.1: An example of the Gallai-Edmonds decomposition of a graph. A maximum matching is shown in red.

The Gallai-Edmonds decomposition of a graph can be found in polynomial time using Edmonds's Blossom algorithm [35, p. 451]. In particular, the problem of deciding whether a graph has a perfect matching is in P. On the other hand, the problem of counting all perfect matchings of a graph is NP-hard, as can be seen in [82, p. 307]. These results and more about matchings in general can be found in Lovász and Plummer's book [82].

The main step in the proof of Theorems A and B is the following result, which appears in [82, p. 95, Lem. 3.2.2].

Theorem C (Stability)**.** *Let G be graph with a vertex i in ∂D_G. Then:*

- $D_{G\setminus i} = D_G$;

- $\partial D_{G\setminus i} = \partial D_G \setminus i$;

- $C_{G\setminus i} = C_G$.

In their work, Ku and Wong [77, p. 3390, Thms. 4.12 and 4.13], based on the work of Godsil [53] and Ku and Chen [71], generalized Theorems A, B and C for the context of weighted matching polynomials. These same theorems have been extensively studied in the particular case of trees with the name Parter-Wiener theory, as can be seen in Johnson and Saiago's book [66, p. 16, Chpt. 2].

Following a line of investigation carried out by Lovász and Plummer [82], Ku and Wong were also able to generalize in the works [72–78] some other classical concepts of matching theory for weighted matching polynomials. Recently, Bencs and Mészáros [15, p. 5-6, Thms. 1.9-1.12] also proved versions of Theorems A, B and C for infinite and random graphs.

Our main result in this section is a refinement of the stability lemma for weighted matching polynomials proved by Ku and Wong. Our proof is simpler and applies graph continued fractions.

Consider graphs with vertex set $[n]$ where the vertex weights are $x - r_i$, with r_i a real number, and the edge weights are non-positive λ_{ij}, so that we are working with weighted matching polynomial. Theorem 17 has the following consequence in this case.

Corollary 28 (Heilmann-Lieb [64]). *All the zeros of the matching polynomial of G are real and contained in the interval $\left[\min_j r_j - 2\sqrt{B_G}, \max_j r_j + 2\sqrt{B_G}\right]$, where B_G is equal to $\max_j \max_{\substack{A\subseteq[n]\setminus j \\ |A|=n-2}} \sum_{k\in A} -\lambda_{jk}$ if $n \geq 3$, and equal to $-\lambda_{12}/4$ or 0 if n is two or one, respectively.*

Proof. As $\mu(G)$ has real coefficients, if it has a non-real zero, then by conjugation it has a zero in the upper half-plane. This is prohibited by Theorem 17, so $\mu(G)$ has only real zeros. The bound on the zeros follows immediately from the second item of Theorem 17. $\square$

The particular case of equal edge weights in Corollary 28 was used by Marcus, Spielman and Srivastava [85, p. 316, Thm. 5.5] in their construction of bipartite Ramanujan graphs of all degrees. The matching polynomials appear in this work as the "average" characteristic polynomial of a random 2-lift of a graph, as can be seen in [85, p. 312-313].

Corollary 28 implies that $\alpha_i(G)(x)$ is a real rational function with all its zeros and poles in the real line. In order to better understand the position of the zeros and poles we look at the derivative of graph continued fractions.

Lemma 29. *Let G be a rooted graph with root i. Then,*

$$\alpha_i(G)'(x) = 1 + \sum_{i\neq j\in[n]} \sum_{c\in[i\to j]} \lambda_c \cdot \left(\frac{\mu(G\setminus c)}{\mu(G\setminus i)}(x)\right)^2 = 1 - \sum_{i\neq j\in[n]} \frac{\lambda_{i\sim j}(x)}{(\alpha_j(G\setminus i)(x))^2}.$$

Proof. Consider the derivative of the recurrence:

$$\alpha_i(G)(x) = x - r_i + \sum_{i \neq j} \frac{\lambda_{ij}}{\alpha_j(G \setminus i)(x)} \implies \alpha_i(G)'(x) = 1 + \sum_{i \neq j} \frac{-\lambda_{ij}\alpha_j(G \setminus i)'(x)}{(\alpha_j(G \setminus i)(x))^2}.$$

Iterating this recurrence for the derivative the result immediately follows.

An alternative proof can be given using the Lemmas 18 and 25, or using the Lemma 21. □

Corollary 30. *Let G be a rooted graph with root i. Then all the zeros and poles of $\alpha_i(G)$ are simple. If θ is not a pole of $\alpha_i(G)$, then $\alpha_i(G)'(\theta) \geq 1$. In particular, $\alpha_i(G)(x)$ is increasing and surjective in each of its branches.*

Proof. If $\mu(G \setminus i)(\theta) \neq 0$, then the Lemma 29 implies that $\alpha_i(G)'(\theta) \geq 1$. It follows by continuity that $\alpha_i(G)'(\theta) \geq 1$ for every θ that is not a pole of $\alpha_i(G)$. In particular, $\alpha_i(G)$ is increasing and surjective in each of its branches and all of its zeros are simple.

Observe that, since $\deg(\mu(G)) = \deg(\mu(G \setminus i)) + 1$, the number of zeros of $\alpha_i(G)$ is one more than the number of poles counted with multiplicity of $\alpha_i(G)$. But in each branch, because $\alpha_i(G)$ is increasing, there can only be one zero of $\alpha_i(G)$. Putting this all together, it follows that all the poles of $\alpha_i(G)$ are also simple. □

Corollary 30 gives a precise picture of how a graph of $\alpha_i(G)(x)$ must look like. In Figure 3.2 we present an example of such a graph.

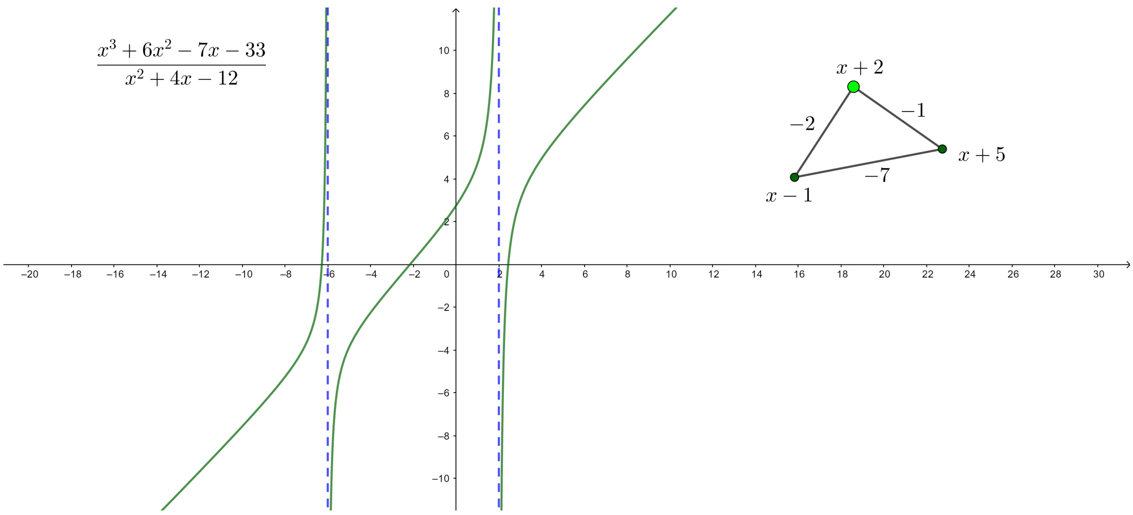


Figure 3.2: An example of a graph of $\alpha_i(G)(x)$.

Corollary 30 also implies the interlacing for the zeros of $\mu(G)$ and $\mu(G \setminus i)$. This result was originally proved by Heilmann and Lieb [64, p. 200, Thm. 4.2]. Denote by $m_\theta(G)$ the multiplicity of θ as a zero of the matching polynomial of G.

Corollary 31 (Interlacing [64])**.** *Let i be a vertex in the graph G. Then $\mu(G)$ and $\mu(G \setminus i)$ interlace, i.e., between any two zeros of $\mu(G)$ there is a zero of $\mu(G \setminus i)$ and vice versa. It is also true that $m_\theta(G \setminus i)$ belongs to $\{m_\theta(G), m_\theta(G) \pm 1\}$ for every real number θ.*

Proof. By Corollary 30 the zeros and poles of $\alpha_i(G)$ are simple. This implies that $m_\theta(G \setminus i)$ belongs to $\{m_\theta(G), m_\theta(G) \pm 1\}$ for every real number θ. The interlacing of the zeros of $\mu(G)$ and $\mu(G \setminus i)$ follows from the interlacing of the zeros and poles of $\alpha_i(G)$ and this last observation about the multiplicities $m_\theta(G)$ and $m_\theta(G \setminus i)$. $\square$

Given a real parameter θ, partition the vertices of the graph G into four sets according to the sign of the graph continued fraction with each vertex as a root. That is, if i is a vertex then:

- $i \in -_{\theta,G}$ if $\alpha_i(G)(\theta)$ is negative;
- $i \in 0_{\theta,G}$ if $\alpha_i(G)(\theta)$ is zero;
- $i \in +_{\theta,G}$ if $\alpha_i(G)(\theta)$ is positive;
- $i \in \infty_{\theta,G}$ if $\alpha_i(G)(\theta)$ is infinite.

This way we have the partition $[n] = -_{\theta,G} \sqcup 0_{\theta,G} \sqcup +_{\theta,G} \sqcup \infty_{\theta,G}$. Define also $\pm_{\theta,G} := -_{\theta,G} \sqcup +_{\theta,G}$. Note that by Corollary 31:

- $i \in 0_{\theta,G}$ if $m_\theta(G \setminus i) = m_\theta(G) - 1$;
- $i \in \pm_{\theta,G}$ if $m_\theta(G \setminus i) = m_\theta(G)$;
- $i \in \infty_{\theta,G}$ if $m_\theta(G \setminus i) = m_\theta(G) + 1$.

It the notation of Ku and Wong in [77, p. 3389-3390]: $0_{\theta,G} = D_{\theta,G}$, $\pm_{\theta,G} = N_{\theta,G}$, $A_{\theta,G} = \partial 0_{\theta,G}$ and $\infty_{\theta,G} \setminus \partial 0_{\theta,G} = P_{\theta,G}$. This shows that the partition $[n] = -_{\theta,G} \sqcup 0_{\theta,G} \sqcup +_{\theta,G} \sqcup \infty_{\theta,G}$ refines the one considered by Ku and Wong in [77, p. 3389], where there was no distinction between $+_{\theta,G}$ and $-_{\theta,G}$.

As observed by Godsil [53, p. 1], if the vertex and edge weights of G are x and -1, respectively, then for θ equal to zero it holds $m_0(G) = def(G)$ and also $0_{0,G} = D_{0,G} = D_G$, $\partial 0_{0,G} = \partial D_{0,G} = \partial D_G$ and $\pm_{0,G} \sqcup (\infty_{0,G} \setminus \partial 0_{0,G}) = N_{0,G} \sqcup P_{0,G} = C_G$. As will be seen later this leads to a generalization of Theorem B.

Looking at Figure 3.2, one can see that as the parameter θ increases from $-\infty$ to $+\infty$ the sign of $\alpha_i(G)(\theta)$ always changes in a prescribed order: $- \to 0 \to + \to \infty \to -$. This already shows that as θ is varied the partitions of $[n]$ change according to some rules. The parameter θ is seen as a time variable determining the values of the graph continued fractions and partitions of $[n]$.

Clearly, if θ is not a zero of $\mu(G)$, then the set $0_{\theta,G}$ is empty. As observed by Godsil [53, p. 5, Lem. 3.1], it turns out that the converse is also true.

Lemma 32 (Godsil [53])**.** *The real number θ is a zero of $\mu(G)$ if, and only if, $0_{\theta,G}$ is non-empty.*

Proof. If θ is a zero of $\mu(G)$, then, by Lemma 25,

$$\infty = \frac{\mu(G)'}{\mu(G)}(\theta) = \sum_{j \in [n]} \frac{\mu(G \setminus j)}{\mu(G)}(\theta) = \sum_{j \in [n]} \frac{1}{\alpha_j(G)(\theta)},$$

which implies that there exists a vertex j satisfying $\alpha_j(G)(\theta) = 0$, i.e., j is in $0_{\theta,G}$. $\square$

The same proof of this last lemma implies:

Lemma 33. *A vertex i is in $\infty_{\theta,G}$ if, and only if, one of its neighbors is in $0_{\theta,G\setminus i}$.*

Proof. Observe that, $\infty = \alpha_i(G)(\theta) = \theta - r_i + \sum_{i\neq j} \frac{\lambda_{ij}}{\alpha_j(G\setminus i)(\theta)}$ if, and only if, there exists a vertex j satisfying $\lambda_{ij} \neq 0$ and $\alpha_j(G\setminus i)(\theta) = 0$, i.e., j is a neighbor of i that belongs to $0_{\theta,G\setminus i}$. □

This last result is best understood using our new interpretation in terms of the path tree. Looking at Figure 3.2, it is clear that that a vertex is in $0_{\theta,G}$ if, and only if, it is in the intersection $-_{\theta-\epsilon,G} \cap +_{\theta+\epsilon,G}$ for every $\epsilon > 0$ sufficiently small. This means that a vertex i is in $0_{\theta,G}$ if, and only if, $\alpha_i(G)(x)$ changes sign from $-$ to $+$ at time θ. A similar reasoning applies for vertices in $\infty_{\theta,G}$.

Using the recurrence $\alpha_i(G)(x) = x - r_i + \sum_{\substack{i\neq j\\ \lambda_{ij}\neq 0}} \frac{\lambda_{ij}}{\alpha_j(G\setminus i)(x)}$, Lemma 33 can be interpreted as saying that $\alpha_i(G)(x)$ changes sign from $+$ to $-$ at time θ if, and only if, for some neighbor j of i, $\alpha_j(G\setminus i)(x)$ changes sign from $-$ to $+$ at time θ.

Consider the path tree T^i_G and write at each level the sign of the graph continued fraction for its respective rooted subtree. That is, for a path $c : i = i_1 \to i_k$ write for the corresponding rooted subtree the sign of $\alpha_{i_k}(G \setminus \{i_1, \ldots, i_{k-1}\})(\theta)$, as shown in Figure 3.3.

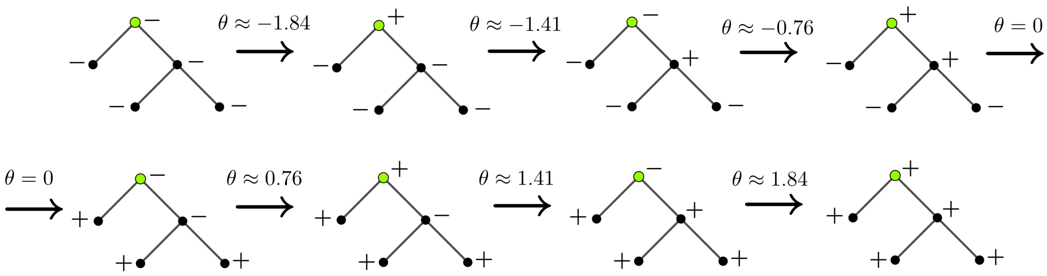


Figure 3.3: A rooted tree with vertex weights x and edge weights -1. The signs are of the graph continued fractions of the subtrees. As time passes the plus signs fill in the tree.

Observe that for large negative times all subtrees have sign $-$, and for large positive times all subtrees have sign $+$. As time goes by the $+$ signs are created at the root of the path tree and descend, sometimes duplicating, but always respecting the rule: a node changes from $+$ to $-$ at time θ if, and only if, one of its sub-nodes changes from $-$ to $+$ at time θ. This is illustrated in Figure 3.3.

It is important to note that the signs in the path tree are not necessarily equal to the signs in the initial graph, i.e., $\alpha_{i_k}(G \setminus \{i_1, \ldots, i_{k-1}\})(\theta)$ is different in general from $\alpha_{i_k}(G)(\theta)$.

The interpretation in terms of the path tree is particularly interesting when studying paths. Let $c : i_1 \to i_k$ be a path in the graph G. Observe that,

$$\frac{\mu(G)}{\mu(G \setminus c)} = \alpha_{i_1}(G)\alpha_{i_2}(G \setminus i_1) \cdots \alpha_{i_k}(G \setminus \{i_1, \ldots, i_{k-1}\}) =$$

$$= \alpha_{i_k}(G)\alpha_{i_{k-1}}(G \setminus i_k) \cdots \alpha_{i_1}(G \setminus \{i_k, i_{k-1}, \ldots, i_2\}).$$

The difference $m_\theta(G) - m_\theta(G \setminus c)$ can be interpreted in terms of the path tree. The multiplicity $m_\theta(G) - m_\theta(G \setminus c)$ is equal to the number of zeros minus the number of infinities for the subtrees of $T_G^{i_1}$ corresponding to the path c. More precisely,

$$m_\theta(G) - m_\theta(G \setminus c) = |\{i_j \in 0_{\theta, G\setminus\{i_1,\ldots,i_{j-1}\}}\}_{j\in[k]}| - |\{i_j \in \infty_{\theta, G\setminus\{i_1,\ldots,i_{j-1}\}}\}_{j\in[k]}| =$$

$$= |\{i_j \in 0_{\theta, G\setminus\{i_k,\ldots,i_{j+1}\}}\}_{j\in[k]}| - |\{i_j \in \infty_{\theta, G\setminus\{i_k,\ldots,i_{j+1}\}}\}_{j\in[k]}|.$$

The second equality corresponds to the same statement but for the reverse path $-c : i_k \to i_1$. In particular, this shows that the difference of zeros and infinities along the path tree coincide for every path and its reverse. As a consequence we have the following result, originally proved by Godsil [53, p. 4-6, Cor. 2.5 and Lem. 3.3].

Lemma 34 (Godsil [53])**.** *Let $c : i \to j$ be a path in the graph G. In this case, $m_\theta(G) - m_\theta(G \setminus c) \leq 1$, and, if there is equality, then both i and j are in $0_{\theta,G}$.*

Proof. Let $c : i_1 \to i_m$ be a path in the graph G. First, notice that whenever there is a zero in a node of the path tree $T_G^{i_1}$ there must be an infinity for the node right above it. In other words, if $\alpha_{i_{k+1}}(G \setminus \{i_1, \ldots, i_k\}) = 0$ for some $k \in [m-1]$, then $\alpha_{i_k}(G \setminus \{i_1, \ldots, i_{k-1}\}) = \infty$. This implies that the number of zeros is less than the number of infinities along the path c in the path tree $T_G^{i_1}$, from which follows that $m_\theta(G) - m_\theta(G \setminus c) \leq 1$.

If the path c satisfies $m_\theta(G) - m_\theta(G \setminus c) = 1$, then, by the same reasoning above, all the infinities along the path c in $T_G^{i_1}$ come from a zero inside the same path c. But there is also one extra zero which does not have a corresponding infinity. Since the extra zero does not have a corresponding infinity, it must be at the root of the path tree $T_G^{i_1}$. This implies that i_1 is in $0_{\theta,G}$. The same reasoning for the reverse path $-c$ implies that i_m is also in $0_{\theta,G}$. $\square$

In Section 3.3 it will be shown that the arguments used in the proof of Lemma 34 naturally lead to a generalization to graph continued fractions of the classical Sturm's theorem [97].

In order to prove the generalization of the Stability Lemma C to graph continued fractions, we must study how a graph continued fraction changes when a vertex is deleted. To approach this problem our main tool is the Contraction Lemma 19.

For distinct vertices i and j it was previously observed that $-\lambda_{i\sim j}$ is a sum of squares. So $\lambda_{i\sim j}(\theta)$ is in $[-\infty, 0]$, but it can happen that $\lambda_{i\sim j}$ is equal to $-\infty$ at time θ. The next proposition, which is a direct consequence of Lemma 34, gives an easily verifiable condition that guarantees $\lambda_{i\sim j}(\theta)$ is finite.

Proposition 35. *If $\lambda_{i\sim j}(\theta) = -\infty$, then $i \in \infty_{\theta, G\setminus j}$ and $j \in \infty_{\theta, G\setminus i}$.*

Proof. Assume i is not in $\infty_{\theta,G}$. In order to verify that $\lambda_{i\sim j}$ is finite it is sufficient to prove that $m_\theta(G \setminus \{i,j\}) \leq m_\theta(G \setminus c)$ for every path c in $[i \to j]$. Consider a path $c : i = i_1 \to i_k = j$ between i and j, and let $\overline{c} : i = i_1 \to i_{k-1}$ be the path in $G \setminus j$ obtained from c.

If i is in $0_{\theta,G\setminus j}$, then, by Lemma 34, it holds, $m_\theta(G \setminus j) - m_\theta(G \setminus (\{j\} \sqcup \overline{c})) \leq 1 \implies$

$$m_\theta(G \setminus \{j,i\}) = m_\theta(G \setminus j) - 1 \leq m_\theta(G \setminus (\{j\} \sqcup \overline{c})) = m_\theta(G \setminus c) \implies$$

$$m_\theta(G \setminus \{i,j\}) \leq m_\theta(G \setminus c).$$

Assume now that the vertex i is in $\pm_{\theta,G\setminus j}$. In this case, by Lemma 34, the path $\overline{c} : i = i_1 \to i_{k-1}$ satisfies $m_\theta(G \setminus j) - m_\theta(G \setminus (\{j\} \sqcup \overline{c})) \leq 0$. This implies that,

$$m_\theta(G \setminus \{j,i\}) - m_\theta(G \setminus c) = m_\theta(G \setminus j) - m_\theta(G \setminus (\{j\} \sqcup \overline{c})) \leq 0 \implies$$

$$m_\theta(G \setminus \{i,j\}) \leq m_\theta(G \setminus c).$$

$\square$

Proposition 36. *If $\lambda_{i\sim j}(\theta) = 0$, then $\alpha_i(G)(\theta) = \alpha_i(G \setminus j)(\theta)$ and $\alpha_j(G)(\theta) = \alpha_j(G \setminus i)(\theta)$.*

Proof. By symmetry it is sufficient to prove the first equality. If $\alpha_j(G \setminus i)(\theta) \neq 0$, then the Contraction Lemma 19 implies $\alpha_i(G)(\theta) = \alpha_i(G \setminus j)(\theta)$. The general case follows from a perturbation argument. Assume that $\alpha_j(G \setminus i)(\theta) = 0$ and consider for a real number r the graph G_r obtained from G where the new vertex weight of j is $x - r_j + r$. If $r \neq 0$, then $\alpha_j(G_r \setminus i)(\theta) = r \neq 0$ and $\lambda_{i\sim j}(\theta) = 0$, and the Contraction Lemma 19 implies that $\alpha_i(G_r)(\theta) = \alpha_i(G_r \setminus j)(\theta) = \alpha_i(G \setminus j)(\theta)$. But then $\alpha_i(G_r)(\theta)$ is a real rational function in r which is equal to $\alpha_i(G \setminus j)(\theta)$ for every real number $r \neq 0$. Thus, equality must also be true at $r = 0$, so $\alpha_i(G)(\theta) = \alpha_i(G_0)(\theta) = \alpha_i(G \setminus j)(\theta)$. $\square$

Proposition 37. *Consider $\lambda_{i\sim j}(\theta) \in (-\infty, 0)$. In this case:*

a) If $i \in +_{\theta,G\setminus j}$ and $j \in +_{\theta,G\setminus i}$, or $i \in -_{\theta,G\setminus j}$ and $j \in -_{\theta,G\setminus i}$, then i and j are simultaneously in either one of $-_{\theta,G}$, $0_{\theta,G}$ or $+_{\theta,G}$;

b) If $i \in +_{\theta,G\setminus j}$ and $j \in -_{\theta,G\setminus i}$, then $i \in +_{\theta,G}$ and $j \in -_{\theta,G}$;

c) If $i \in 0_{\theta,G\setminus j}$ and $j \in 0_{\theta,G\setminus i}$, then $i, j \in \infty_{\theta,G}$;

d) If $i \in 0_{\theta,G\setminus j}$ and $j \in +_{\theta,G\setminus i}$, then $i \in -_{\theta,G}$ and $j \in \infty_{\theta,G}$;

e) If $i \in 0_{\theta,G\setminus j}$ and $j \in -_{\theta,G\setminus i}$, then $i \in +_{\theta,G}$ and $j \in \infty_{\theta,G}$;

f) If $i \in \infty_{\theta,G\setminus j}$, then $\alpha_j(G \setminus i)(\theta) = \alpha_j(G)(\theta)$ and $i \in \infty_{\theta,G}$.

Proof. Consider $i \in +_{\theta,G\setminus j}$ and $j \in +_{\theta,G\setminus i}$, the other cases being analogous. The Contraction Lemma 19 implies that $\alpha_i(G)(\theta) = \alpha_i(G \setminus j)(\theta) + \dfrac{\lambda_{i\sim j}(\theta)}{\alpha_j(G \setminus i)(\theta)}$ and $\alpha_j(G)(\theta) = \alpha_j(G \setminus i)(\theta) + \dfrac{\lambda_{j\sim i}(\theta)}{\alpha_i(G \setminus j)(\theta)}$. It then follows that $\alpha_i(G)(\theta)$ and $\alpha_j(G)(\theta)$ are both finite and have the same sign. This shows that i and j are simultaneously in either one of $-_{\theta,G}$, $0_{\theta,G}$ or $+_{\theta,G}$. $\square$

Proposition 38. *Let $\lambda_{i\sim j}(\theta) \in (-\infty, 0)$. In this case:*

a) If $i \in +_{\theta,G\setminus j} \cap +_{\theta,G}$ and $j \in +_{\theta,G\setminus i} \cap +_{\theta,G}$, then $0 < \alpha_i(G)(\theta) < \alpha_i(G \setminus j)(\theta)$ and $0 < \alpha_j(G)(\theta) < \alpha_j(G \setminus i)(\theta)$;

b) If $i \in -_{\theta,G\setminus j} \cap -_{\theta,G}$ and $j \in -_{\theta,G\setminus i} \cap -_{\theta,G}$, then $\alpha_i(G \setminus j)(\theta) < \alpha_i(G)(\theta) < 0$ and $\alpha_j(G \setminus i)(\theta) < \alpha_j(G)(\theta) < 0$;

c) If $i \in +_{\theta,G\setminus j} \cap +_{\theta,G}$ and $j \in -_{\theta,G\setminus i} \cap -_{\theta,G}$, then $\alpha_i(G \setminus j)(\theta) < \alpha_i(G)(\theta)$ and $\alpha_j(G)(\theta) < \alpha_j(G \setminus i)(\theta)$.

Proof. The proof uses the Contraction Lemma 19 and is analogous to that of Proposition 37. $\square$

Proposition 39. *If $\lambda_{i\sim j}(\theta) = -\infty$, then i and j are simultaneously in either one of $-_{\theta,G}$, $0_{\theta,G}$, $+_{\theta,G}$ or $\infty_{\theta,G}$.*

Proof. If $\lambda_{i\sim j}(\theta) = -\infty$, then Proposition 35 implies $i \in \infty_{\theta,G\setminus i}$ and $j \in \infty_{\theta,G\setminus i}$. It follows that $i \in +_{\theta-\epsilon,G\setminus j} \cap -_{\theta+\epsilon,G\setminus j}$ and $j \in +_{\theta-\epsilon,G\setminus i} \cap -_{\theta+\epsilon,G\setminus i}$ for every $\epsilon > 0$ sufficiently small. Since $\lambda_{i\sim j}(\theta - \epsilon) \neq -\infty$, $i \in +_{\theta-\epsilon,G\setminus j}$ and $j \in +_{\theta-\epsilon,G\setminus i}$, the item (a) of Proposition 37 implies that $\alpha_i(G)(\theta - \epsilon)$ and $\alpha_j(G)(\theta - \epsilon)$ have the same sign for every $\epsilon > 0$ small. Similarly, $\alpha_i(G)(\theta + \epsilon)$ and $\alpha_j(G)(\theta + \epsilon)$ have the same sign for every $\epsilon > 0$ small. As a consequence, $\alpha_i(G)(\theta)$ and $\alpha_j(G)(\theta)$ have the same sign, which finishes the proof. $\square$

The content of Propositions 35, 36, 37, 38 and 39 is summarized in Figure 3.4.

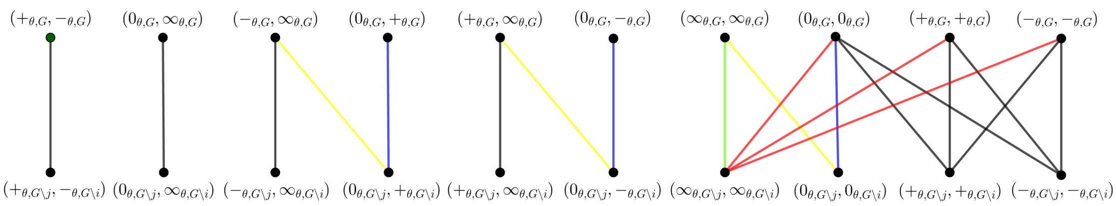


Figure 3.4: The nodes represent possible signs for the pair of distinct vertices (i, j), both in G and in $G \setminus j$ and $G \setminus i$. The edges join signs configurations that can occur simultaneously. The green, black and yellow edges represent $\lambda_{i\sim j}$ in $[-\infty, 0]$, $(-\infty, 0]$ and $(-\infty, 0)$, respectively. The red and blue edges represent $\lambda_{i\sim j}$ equal to $-\infty$ and 0, respectively.

Proposition 40. *The frontier $\partial 0_{\theta,G}$ is a subset of $\infty_{\theta,G}$.*

Proof. Let i be in $\partial 0_{\theta,G}$ with a neighbor j in $0_{\theta,G}$. Since i and j are neighbors, $\lambda_{i\sim j}(\theta)$ is non-zero. By Proposition 37 this implies that i cannot be in $\pm_{\theta,G}$, so it must be in $\infty_{\theta,G}$. $\square$

Corollary 41. *Let i and j be neighbors in the graph G. If $\alpha_i(G)$ changes sign from $-$ to $+$ at time θ, then $\alpha_j(G)$ changes sign from $-$ to $+$ or from $+$ to $-$ at time θ.*

Proof. If $\alpha_i(G)$ changes sign from $-$ to $+$ at time θ, then $i \in 0_{\theta,G}$. This implies by Proposition 40 that $j \in 0_{\theta,G} \sqcup \infty_{\theta,G}$, from which the result follows. $\square$

Proposition 42. *If $i \in \partial 0_{\theta,G}$ and $j \in \pm_{\theta,G}$ then $\alpha_j(G \setminus i)(\theta) = \alpha_j(G)(\theta)$. As a consequence, $-_{\theta,G\setminus i} = -_{\theta,G}$ and $+_{\theta,G\setminus i} = +_{\theta,G}$.*

Proof. Let $k \in 0_{\theta,G}$ be a neighbor of $i \in \partial 0_{\theta,G}$. By Propositions 35, 36, 37, 39 and 38 (or Figure 3.4), since $j \in \pm_{\theta,G}$, it holds that $k \in 0_{\theta,G\setminus j}$ and $i \notin 0_{\theta,G\setminus j}$. But the vertices k and i are also neighbors in $G \setminus j$, and from Proposition 40 we have $\partial 0_{\theta,G\setminus j} \subseteq \infty_{\theta,G\setminus j}$, so it must be $i \in \infty_{\theta,G\setminus j}$. Using item (f) of Proposition 37 the result immediately follows. $\square$

Now we are ready to prove our main result, a refined version of the Stability Lemma C for graph continued fractions.

Theorem 43 (Stability for graph continued fractions)**.** *Let i be a vertex in $\partial 0_{\theta,G}$. Then $\alpha_j(G \setminus i)(\theta) = \alpha_j(G)(\theta)$ for every j different from i. In particular:*

- $-_{\theta,G\setminus i} = -_{\theta,G}$;
- $0_{\theta,G\setminus i} = 0_{\theta,G}$;
- $+_{\theta,G\setminus i} = +_{\theta,G}$;
- $\infty_{\theta,G\setminus i} = \infty_{\theta,G} \setminus i$.

Proof. Consider i in $\partial 0_{\theta,G}$. By Proposition 42 we need to prove the second and fourth equalities of sets. From Propositions 35, 36, 37, 39, 38 and 42 it is clear that $0_{\theta,G} \subseteq 0_{\theta,G\setminus i}$ and $\infty_{\theta,G\setminus i} \subseteq \infty_{\theta,G}$, but it could happen that the intersection $0_{\theta,G\setminus i} \cap \infty_{\theta,G}$ is non-empty.

Assume, by contradiction, that there exists a vertex j in $0_{\theta,G\setminus i} \cap \infty_{\theta,G}$ and let $k \in 0_{\theta,G}$ be a neighbor of i. Consider the graph G_ϵ obtained from G where the new vertex weight of i is $x - r_i + \epsilon$, with $\epsilon > 0$ small. As $i \in 0_{\theta,G\setminus j} \cap \infty_{\theta,G}$ it follows that $i \in +_{\theta,G_\epsilon\setminus j} \cap \infty_{\theta,G_\epsilon}$. By Propositions 35, 36, 37, 39 and 38 this implies that $j \in 0_{\theta,G_\epsilon\setminus i} \cap -_{\theta,G_\epsilon}$ and $k \in 0_{\theta,G_\epsilon\setminus i} \cap 0_{\theta,G_\epsilon}$. Since $j \in -_{\theta,G_\epsilon}$ the Propositions 35, 36, 37 imply that $k \in 0_{\theta,G_\epsilon\setminus j}$. Thus, $i \in +_{\theta,G_\epsilon\setminus j}$ is a neighbor of $k \in 0_{\theta,G_\epsilon\setminus j}$ in $G_\epsilon \setminus j$, which is a contradiction by Proposition 40. $\square$

A graph G is called θ-critical if $[n] = 0_{\theta,G}$. The θ-critical components of a graph G are the connected components of the induced subgraph in $0_{\theta,G}$. In this context there is the following analogue of Theorem A proved by Ku and Wong [77, p. 3390, Thm. 4.13].

Theorem 44 (Gallai's lemma analogue by Ku and Wong [77]). *If G is a connected θ-critical graph then $m_\theta(G) = 1$.*

Proof. Assume, by contradiction, that $[n] = 0_{\theta,G}$ and $m_\theta(G)$ is at least two. Consider a vertex i in $[n] = 0_{\theta,G}$. In this case, since $m_\theta(G \setminus i) \geq 1$, the Lemma 32 implies that $0_{\theta,G\setminus i}$ is non-empty. As i does not belong to $\infty_{\theta,G}$, the Lemma 33 implies that the neighbors of i are not in $0_{\theta,G\setminus i}$. Since the graph G is connected, there exists a path from some neighbor of i to a vertex in $0_{\theta,G\setminus i}$. This shows that $\partial 0_{\theta,G\setminus i}$ is non-empty.

Let j be a vertex in $\partial 0_{\theta,G\setminus i}$. In particular, by Proposition 40, $j \in \infty_{\theta,G\setminus i}$. As $j \in \infty_{\theta,G\setminus i} \cap 0_{\theta,G}$ and $i \in 0_{\theta,G}$, we have by Propositions 37 and 38 that $i \in \infty_{\theta,G\setminus j}$. This implies by Lemma 33 that there exists a neighbor k of i that is in $0_{\theta,G\setminus\{j,i\}}$. But by the Stability Lemma 43 applied to $j \in \partial 0_{\theta,G\setminus i}$ it holds that $0_{\theta,G\setminus i,j} = 0_{\theta,G\setminus i}$. Thus the neighbor k of i is in $0_{\theta,G\setminus i}$, which implies by Lemma 33 that i is in $\infty_{\theta,G}$, reaching a contradiction. ☐

A graph is *vertex-transitive* if for every pair of vertices i and j there exists an automorphism of the graph that maps i to j. Informally speaking, a graph is vertex-transitive if it is the same from the point of view of each vertex. Theorem 44 has the following corollary for vertex-transitive graphs, which was proved by Ku and Chen [71, p. 121, Cor. 1.8].

Corollary 45 (Ku, Chen [71]). *Let G be a connected vertex-transitive graph with vertex weights x and edge weights -1. Then the matching polynomial of G has distinct zeros.*

Proof. Let θ be a zero of the matching polynomial of G. By Lemma 32 the set $0_{\theta,G}$ is non-empty. Let i be a vertex in $0_{\theta,G}$. As G is vertex-transitive, for each vertex j the graphs $G \setminus j$ and $G \setminus i$ are isomorphic. Since the vertex and edge weights are all x and -1, respectively, this implies that $\mu(G \setminus j) = \mu(G \setminus i)$ for each vertex j. As a consequence, for every vertex j it holds $\alpha_j(G) = \dfrac{\mu(G)}{\mu(G \setminus j)} = \dfrac{\mu(G)}{\mu(G \setminus i)} = \alpha_i(G) \in 0_{\theta,G}$, from which follows that j is in $0_{\theta,G}$. This proves that all vertices of G are in $0_{\theta,G}$, i.e., G is θ-critical. Since G is connected and θ-critical it follows by Theorem 44 that θ is a simple zero of the matching polynomial of G. Since all zeros of $\mu(G)$ are simple, we conclude that $\mu(G)$ has distinct zeros. ☐

In contrast to the result of the Theorem 45 for the matching polynomial, the characteristic polynomial of any vertex-transitive graph with more than two vertices has multiple zeros [16, p. 117, Thm. 15.4].

Corollary 45 was one of the motivations for the development of Theorem 44. The reason for this is the following conjecture of Lovász [81].

Conjecture 46 (Lovász [81]). *Every finite connected vertex-transitive graph contains a Hamiltonian path.*

Although Conjecture 46 is traditionally stated in a positive tone, it is wide open and it seems there is no consensus as to whether one should believe it to be true. Currently, the best result in the direction of this conjecture that applies for all vertex-transitive graphs is in Babai's work [10, p. 302, Thm.].

Theorem 47 (Babai [10]). *Every finite connected vertex-transitive graph with $n \geq 4$ vertices contains a cycle of length at least $\sqrt{3n}$.*

As explained in the work of Godsil [53, p. 2], if Conjecture 46 turns out to be true, then Corollary 45 immediately follows. This happens because, by a result of Godsil [50, p. 296, Cor. 5.3], if a graph contains a path of length l, then its matching polynomial has at least $l + 1$ zeros. The connection between paths and matching polynomials will be the main theme of Sections 3.3 and 3.4 and of Chapter 4 of this thesis.

The Theorem 44 also leads to the following corollary by Ku and Wong [77, p. 3409, Cor. 4.14].

Corollary 48 (Ku, Wong [77]). *The multiplicity of θ as a zero of $\mu(G)$ is equal to the number of θ-critical components of G minus the number of vertices in $\partial 0_{\theta,G}$.*

Proof. Note that by the Stability Lemma 43 the θ-critical components of $G \setminus \partial 0_{\theta,G}$ are the θ-critical components of G. But in $G \setminus \partial 0_{\theta,G}$ all the θ-critical components are isolated. This implies by Theorem 44 that $m_\theta(G \setminus \partial 0_{\theta,G})$ is equal to the number of θ-critical components of G. By the Stability Lemma 43 it also holds that $m_\theta(G \setminus \partial 0_{\theta,G})$ is equal to $m_\theta(G) + |\partial 0_{\theta,G}|$, from which the result readily follows. $\square$

The Corollary 48 implies that if θ is a zero of $\mu(G)$, then, since $m_\theta(G) \geq 1$, there are more θ-critical components of G than there are vertices in $\partial 0_{\theta,G}$. It turns out that the analogue of item (c) of the Gallai-Edmonds Structure Theorem B holds for matching polynomials.

Corollary 49. *For every subset S of $\partial 0_{\theta,G}$ there are at least $|S| + 1$ θ-critical components of G that are connected to a vertex in S.*

Proof. By the Stability Lemma 43 we can restrict ourselves to the graph G' obtained from G by first deleting all the vertices in $\partial 0_{\theta,G} \setminus S$ and then deleting all the isolated θ-critical components. Observe that $\partial 0_{\theta,G'} = S$ and all the θ-critical components of G' are θ-critical components of G. Since $m_\theta(G') \geq 1$ and $\partial 0_{\theta,G'} = S$, the Corollary 48 implies that there at least $|S| + 1$ θ-critical components in G'. But there are no isolated θ-critical components in G', so all of the $|S| + 1$ θ-critical components are connected to a vertex in S. $\square$

Using Corollary 49 and the path tree we can give a new conceptual explanation for why the Stability Lemma 43 is true. Let i and $j \in \partial 0_{\theta,G}$ be two distinct vertices of the graph G and consider the tree continued fraction $\alpha_i(T_G^i)(\theta)$. Observe that for every path $c : i = i_1 \to i_k = j$ it holds $\alpha_j(G \setminus \{i_1, \ldots, i_{k-1}\})(\theta) = \infty$. This means that along the tree continued fraction $\alpha_i(T_G^i)(\theta)$, the vertex j always corresponds to a node with an infinity, and so it can be disregarded.

In order to see this, note that if the path c does not go through $0_{\theta,G}$, then by Propositions 35, 36, 37, 38 and 39 (or Figure 3.4) the original θ-critical components are unaffected. It follows that there is a remaining θ-critical component connected to j which guarantees $\alpha_j(G \setminus \{i_1, \ldots, i_{k-1}\})(\theta) = \infty$. Now, if the path c goes through $0_{\theta,G}$, then the Corollary 49 guarantees that in this case there is also a remaining θ-critical component connected to j forcing it to be in $\infty_{\theta,G \setminus \{i_1,\ldots,i_{k-1}\}}$.

With this same reasoning, it is clear that the following new version of the Stability Theorem 43 is also true.

Theorem 50 (Stability lemma II)**.** *Let G be a graph with two distinct vertices i and $j \in \partial 0_{\theta,G}$. Consider the graph G' obtained from G where the weights r_j and $\lambda_{jk} \leq 0$, for all $k \neq j$, are modified. Assume that for every subset S of $\partial 0_{\theta,G}$ there are at least $|S|+1$ θ-critical components of G that are connected to a vertex in S in the graph G'. In this case, $\alpha_i(G')(\theta) = \alpha_i(G)(\theta)$ for every vertex i.*

Using the techniques presented in this section it is possible to give new proofs and refinements for other results presented in the works of Ku and Wong [72–78].

It is also interesting to note that the Stability Theorem 43 basically follows from the Contraction Lemma 19. As this last lemma is a consequence of the Christoffel-Darboux Lemma 18, and there is the corresponding Lemma 4 for characteristic polynomials, there is some kind of analogue of the Theorem 43 for characteristic polynomials. The works by Van Mieghem [86] and by Johnson and Saiago [66] study how the characteristic polynomial of a graph changes when a vertex is deleted.

In 2020, Banks, Garza-Vargas and Mukherjee [11] presented a result very close to the Gallai-Edmonds structure decomposition for weighted matching polynomials. In their work, they investigated the atoms of the universal cover measure of a weighted graph.

The *universal covering* of a connected weighted graph G is the unique (up to isomorphism) weighted infinite tree that is a covering of every other covering of G, where the weights are assigned in the obvious way. The *universal covering measure* of G is the spectral measure of its universal covering. The work of Bordenave and Collins [18] shows that the universal covering measure controls to some extent the spectrum of random lifts of a weighted graph G. Random lifts are useful in constructing *expander graphs* as seen in the articles by Marcus, Spielman and Srivastava [85] and by O'Donnell and Wu [88].

Building on the work of Aomoto [6,7], Banks, Garza-Vargas and Mukherjee [11, p. 8-9, Thms. 3.1-3.3] proved a structural result for atoms of the universal covering measure analogous to the Gallai-Edmonds decomposition studied in this section. In short, the work [11] presents situation analogous to this section where the path tree is replaced by universal covering.

As a consequence of their structural result, Banks, Garza-Vargas and Mukherjee [11, p. 8, Thms. 3.2] obtained that the atoms of the universal covering measure are also zeros of the characteristic polynomial of the initial graph. In particular, this gives a finite time algorithm [11, p. 9, Cor. 3.1] to compute the atoms of the universal covering measure.

Although not noted in their work, their results imply that the atoms of the universal covering measure are also zeros of the matching polynomial of the initial graph. More generally, these atoms are zeros of every μ-polynomial, which is a common generalization of the characteristic and matching polynomials defined in the work of Gutman and Polansky [62, p. 207]. This class of polynomials is also considered in another paper by Gutman [58, p. 58, Thms. 1 and 2].

It also appears that the finite time algorithm for calculating the atoms of the universal covering measure described in [11, p. 9, Cor. 3.1] can be improved using the structure decomposition for characteristic polynomials alluded to above. For example, to determine whether 0 is an atom of the universal covering measure, one can use the classical Gallai-Edmonds Structure Theorem B.

Also noteworthy are the recent work by Garza-Vargas and Kulkarni [48], which study the universal covering measure from the viewpoint of the theory of *free probabilities*, and the independent work by Simon, Avni, Breuer, Christiansen, Zinchenko and Kalai [8, 9, 25] that studies the universal covering measure with the aim of generalizing the theory of *periodic Schrödinger operators in one dimension*. Finally, in Aomoto's work [5, p. 306] the theory of periodic continued fractions is already mentioned in connection to the universal covering measure.

These connections are being investigated and will be the subject of our future work.

3.2 Lower Bound for the Largest Zero of a Matching Polynomial

Using the techniques from the last section, we can also prove an easy lower bound for the largest zero of a matching polynomial in the same spirit as the Heilmann-Lieb Theorem 28. The second part of the next lemma appears in Godsil and Gutman's work [56, p. 143].

Lemma 51. *Let G be a connected graph. If θ is the largest or smallest zero of $\mu(G)$, then G is θ-critical. In particular, θ is a simple zero of $\mu(G)$.*

Proof. Let θ be the smallest zero of $\mu(G)$. By Proposition 32 we know that $0_{\theta,G}$ is non-empty. Observe that, if x is smaller than θ, then $[n] = -_{x,G}$. This implies that at time θ all the vertices are in $-_{\theta,G} \sqcup 0_{\theta,G}$. But G is connected and by Proposition 40 it holds $\partial 0_{\theta,G} \subseteq \infty_{\theta,G}$, so it must be $[n] = 0_{\theta,G}$. This implies, by Theorem 44 that $m_\theta(G) = 1$, so θ is a simple zero. For the largest zero of $\mu(G)$ the proof is analogous. $\square$

Given a graph G denote by z_G the largest zero of its matching polynomial.

Lemma 52. *Let G be a connected graph and consider the graph G' obtained from G where the edge ij receives a new weight $\lambda_{ij} < \lambda'_{ij} \leq 0$. In this case, $z_G > z_{G'}$.*

Proof. The Lemma 51 shows that G is z_G-critical. Using the interlacing of Corollary 31 this implies that the largest zero of $\mu(G \setminus \{i,j\})$ is smaller than z_G. It follows that $\mu(G)(x) \geq 0$ and $\mu(G \setminus \{i,j\})(x) > 0$ for $x \geq z_G$. As a consequence, $\mu(G')(x) = \mu(G)(x) - (\lambda_{ij} - \lambda'_{ij})\mu(G \setminus \{i,j\})(x) > 0$, for $x \geq z_G$. This shows that the largest zero of $\mu(G')$ is smaller than the largest zero of $\mu(G)$. $\square$

Lemma 53. *Let G be a connected graph with at least three vertices and $r_i = \max_j r_j$. In this case,*

$$r_i < z^* \leq z_G < r_i + 2\sqrt{\max_j \max_{\substack{A\subseteq[n]\setminus j\\ |A|=n-2}} \sum_{k\in A} -\lambda_{jk}},\ \textit{where } z^* = r_i + \sum_{j\neq i} \frac{-\lambda_{ij}}{z^* - r_j}.$$

In particular, if r_j is zero for every j, then,

$$\sqrt{\max_j \sum_{k\neq j} -\lambda_{jk}} \leq z_G < 2\sqrt{\max_j \max_{\substack{A\subseteq[n]\setminus j\\ |A|=n-2}} \sum_{k\in A} -\lambda_{jk}}.$$

Proof. The upper bound for z_G comes from Corollary 28 and the fact that G has at least three vertices. For the lower bound consider the graph G' obtained from G where all the edges that are not incident to i are set to zero. By Lemma 52 the largest zero of $\mu(G')$, denoted by z^*, is less than or equal to z_G. As i is not an isolated vertex in G' the Lemma 52 implies that z^* is bigger than r_i. Finally, observe that,

$$\mu(G')(x) = \prod_j (x - r_j) + \sum_{j\neq i} \lambda_{ij} \prod_{k\neq i,j} (x - r_k) \implies$$

$$\prod_j (z^* - r_j) = \sum_{j\neq i} -\lambda_{ij} \prod_{k\neq i,j} (z^* - r_k) \implies z^* - r_i = \sum_{j\neq i} \frac{-\lambda_{ij}}{z^* - r_j}.$$

□

3.3 Depth-First Search Trees and Sturm's Theorem

In this section, we obtain a new generalization for graph continued fractions of the following modification by Sylvester [98] of the classical Sturm's theorem [97] (or see [69, p. 305, Thm. 7.10]) about the number of zeros of a real polynomial in an interval.

Consider two monic real polynomials p and q of degrees n and $n-1$, respectively, with real and distinct zeros. Assume that the zeros of p and q are different and interlace. In particular, one can take q as the derivative of p divided by n, so that p and q are monic and interlace. It is known, as will be seen in Section 4.2, that performing the Euclidean algorithm for p and q results in:

$$\frac{p}{q}(x) = x - r_1 + \cfrac{\lambda_1}{x - r_2 + \cfrac{\lambda_2}{\ddots + \cfrac{\lambda_{n-1}}{x - r_n}}},$$

where r_i is a real number and λ_i is negative for every i. The sequence of partial numerators of this continued fraction is known as the Sturm sequence for the pair (p, q) and is the starting segment of an orthogonal polynomial sequence, which will be the subject of Section 4.1.

Denote by $\tau_i(x)$ and $\hat{\tau}_i(x)$, for every i in $[n]$, the continued fractions,

$$\tau_i(x) := x - r_i + \cfrac{\lambda_i}{x - r_{i+1} + \cfrac{\lambda_{i+1}}{\ddots + \cfrac{\lambda_{n-1}}{x - r_n}}}, \quad \hat{\tau}_i(x) := x - r_i + \cfrac{\lambda_{i-1}}{x - r_{i-1} + \cfrac{\lambda_{i-2}}{\ddots + \cfrac{\lambda_1}{x - r_1}}}.$$

Note that except for a finite number of values of θ it holds $\tau_i(\theta), \hat{\tau}_i(\theta) \in \mathbb{R} \setminus \{0\}$ for every i in $[n]$. Let θ be a real number with this property, and denote by $V(\theta)$ and $\hat{V}(\theta)$ the number of positive terms among $\tau_1(\theta), \tau_2(\theta), \ldots, \tau_n(\theta)$ and $\hat{\tau}_1(\theta), \hat{\tau}_2(\theta), \ldots, \hat{\tau}_n(\theta)$, respectively.

In this case, there is the following version by Sylvester [98] of Sturm's theorem.

Theorem D (Sylvester modification of Sturm's theorem [98])**.** *Both $V(\theta)$ and $\hat{V}(\theta)$, when defined, are equal to the number of zeros of $p(x)$ in the interval $(-\infty, \theta)$.*

First, we show how this theorem can be easily generalized to graph continued fractions when the graph has a Hamiltonian path.

Consider a path $c : i_1 \to i_k$ in the graph G. Recall, from Section 3.1, that for every real number θ the multiplicity $m_\theta(G) - m_\theta(G \setminus c)$ can be interpreted by counting zeros and infinities along the path $c : i_1 \to i_k$ in the path tree $T_G^{i_1}$. This fact was used, in particular, to verify that $m_\theta(G) - m_\theta(G \setminus c) \leq 1$ in Lemma 34.

Observe that, except for a finite number of times θ, there are only plus and minus signs along the path c in $T_G^{i_1}$. In this case, there is also an interpretation for the number of plus signs along the path $c : i_1 \to i_k$ in $T_G^{i_1}$.

Note that the total variation of the number of plus signs along c in $T_G^{i_1}$ at time θ is equal to $m_\theta(G) - m_\theta(G \setminus c)$. Since for a large negative time all subtrees of the path tree have negative signs, it follows that, except for finite number of times θ,

$$\sum_{x<\theta} (m_x(G) - m_x(G \setminus c)) = |\{i_j \in +_{\theta, G\setminus\{i_1,\ldots,i_{j-1}\}}\}_{j\in[k]}|.$$

For this reason we call $m_\theta(G) - m_\theta(G \setminus c)$ the *entry* (of plus signs) at time θ in the path c in $T_G^{i_1}$. The fact $m_\theta(G) - m_\theta(G \setminus c) \leq 1$, proved in Lemma 34, means that the entry at time θ in c is at most one. This is clear because the plus signs can only enter c through the root of $T_G^{i_1}$. If c has entry equal to one at time θ, then the Lemma 34 and its proof imply that no plus sign escapes c and there is a new plus sign that enters through the root of $T_G^{i_1}$ at time θ.

Also, since $\mu(G \setminus c)$ is the same as $\mu(G \setminus -c)$, the entry of c is equal to the entry of the reverse path $-c$ for every time θ.

Denote by $V_c(\theta)$ the number of plus signs along the path c in the path tree $T_G^{i_1}$ at a time θ such that there are only plus or minus signs, i.e., $V_c(\theta) = |\{i_j \in +_{\theta, G\setminus\{i_1,\ldots,i_{j-1}\}}\}_{j\in[k]}|$. Since a path and its reverse have the same entry at all times, it follows that $V_c(\theta)$ is equal to $V_{-c}(\theta)$, for every θ. Putting it all together, there is the following new result.

Theorem 54 (Sturm's theorem for paths)**.** *Let c be a path in the graph G. Then, both $V_c(\theta)$ and $V_{-c}(\theta)$, when defined, are equal to,*

$$\sum_{x<\theta} m_x(G) - m_x(G \setminus c).$$

In case the path is Hamiltonian, we obtain the following new generalization of Sylvester's version of Sturm's Theorem D.

Corollary 55 (Sturm's theorem for Hamiltonian paths)**.** *Let c be a Hamiltonian path in the graph G. Then, $\mu(G)$ has distinct zeros and both $V_c(\theta)$ and $V_{-c}(\theta)$, when defined, are equal to the number of zeros of $\mu(G)$ in the interval $(-\infty, \theta)$.*

Proof. Note that because c is Hamiltonian, it follows that $G \setminus c = \emptyset$. Now, $m_\theta(G) = m_\theta(G) - m_\theta(G \setminus c)$ is the entry of c at time θ and so it is at most one by the previous observations. This shows that $m_\theta(G)$ is one for every zero θ of $\mu(G)$, and as a consequence $\mu(G)$ has distinct zeros.

By Theorem 54, it also follows that $\sum_{x<\theta} m_x(G)$ is equal to both $V_c(\theta)$ and $V_{-c}(\theta)$, when defined. As $\mu(G)$ has distinct zeros, the sum $\sum_{x<\theta} m_x(G)$ is equal to the number of zeros of $\mu(G)$ in the interval $(-\infty, \theta)$. □

As the Theorem 54 was obtained by counting plus signs along a path, this leads to the question of whether a similar theorem holds true by counting along subtrees. This is the case for a class of subtrees that can be obtained using the depth-first search algorithm.

Depth-first search (DFS) is an algorithm used to traverse a connected graph. The algorithm starts at a root vertex and explores as far as possible along each path before backtracking. The output of this algorithm is a rooted *spanning tree* of the graph, i.e., a rooted subtree which contains all the vertices of the graph.

The algorithm runs as follows. Consider a connected graph G with n vertices. After the k-th step of the algorithm we have a subtree T_k of G with root i_1 and vertices $\{i_1, \ldots, i_k\}$. To start with, choose some vertex i_1 of G and consider the trivial rooted subtree T_1 of G which consists of the single vertex i_1. If k is smaller than n, then at the $(k+1)$-th step of the algorithm one obtains a new subtree T_{k+1} from the subtree T_k by the following rule. Let j be the largest element in $[k]$ such that i_j has a neighbor which is not in T_k. Since G is connected this element always exists. Declare i_{k+1} as one of the neighbors of i_j which is not in T_k and define the rooted tree T_{k+1} as T_k plus the vertex i_{k+1} and the edge $i_j i_{k+1}$. At the last step of the algorithm one obtains the rooted spanning tree T_n of G with root i_1.

More information about the depth-first search algorithm can be found in the book [82, p. 55]. For this work, the important part is a property that characterizes the spanning trees obtained in the intermediate steps of this algorithm. We present a list of results with immediate properties of DFS-trees that are certainly well known.

Given a vertex j in a rooted tree T denote by $\bar{c}_{T,j}$ the unique path from the root to j, and by $c_{T,j}$ the path $\bar{c}_{T,j}$ minus its last vertex j. The vertex k is a *son* of j if j is the endpoint of the path $c_{T,k}$. In this setting we have the following definition.

Definition 56 (Partial DFS-tree)**.** *A rooted subtree T of the graph G is a partial DFS-tree if for every vertex j in T all of its sons are in different connected components of $G \setminus \bar{c}_{T,j}$. If the partial DFS-tree is also a spanning tree, then it is called a DFS-tree.*

Observe that every path in a graph corresponds to a partial DFS-tree, and a path is Hamiltonian if, and only if, it corresponds to a DFS-tree.

Proposition 57 (DFS-trees and the depth-first search algorithm)**.** *The rooted trees obtained in the intermediate steps of a depth-first search algorithm are partial DFS-trees. In particular, the output of a depth-first search is a DFS-tree. Conversely, every DFS-tree is the output of a depth-first search.*

Proof. First, we prove by induction on k that all intermediate trees T_k, for k in $[n]$, of a depth-first search are partial DFS-trees. Assume that T_k is a partial DFS-tree and consider the vertex i_j in T_k which is connected to i_{k+1} in T_{k+1}. Observe that, since T_k is a partial DFS-tree by induction hypothesis, we only need to check the definition of partial DFS-tree for the vertex i_j in the tree T_{k+1}. In fact, if we can prove that i_{k+1} is not in the same connected component as i_r in the graph $G \setminus T_j$ for $j < r < k+1$, then the induction step is valid. But, if this was not the case, then it would follow that there exists a vertex i_r for some $j < r < k+1$ with a neighbor which is not in T_k, which is impossible by the definition of i_{k+1}. This proves the induction step and the first part of the statement.

For the second part assume that T is a DFS-tree in the graph G, we want to show that T is the output of a depth-first search in the graph G. First, perform a depth-first search in the tree T starting at its root. The output of this algorithm is the rooted tree T itself and an enumeration $\{i_1, \ldots, i_n\}$ of its vertices where i_1 is the root. We claim that by following the enumeration of the vertices $i_1, \ldots, i_n$ we are also performing a depth-first search in the graph G, which has the tree T as output. To prove this, we need to show that if i_{k+1} is connected to i_j in the tree T with j smaller than k, then no vertex i_r with $j < r \leq k$ has a neighbor in $\{i_{k+1}, \ldots, i_n\}$ in the graph G. In fact, if this were not the case, then it would follow that there exists neighboring vertices i_r and i_s in the graph G with $j < r \leq k$ and $k+1 \leq s \leq n$. Since no vertex in $\{i_{j+1}, \ldots, i_k\}$ has a neighbor in $\{i_{k+1}, \ldots, i_n\}$ in the tree T, it follows that there is a last common point i_t of the paths $\overline{c}_{T,i_r}$ and $\overline{c}_{T,i_s}$ which is contained in $\{i_1, \ldots, i_j\}$. But then, since $i_r i_s$ is an edge in the graph G, it follows that two sons of i_t are in a same connected component of $G \setminus \overline{c}_{T,i_t}$, which is impossible because T is a DFS-tree. This shows that no vertex i_r with $j < r \leq k$ has a neighbor in $\{i_{k+1}, \ldots, i_n\}$ in the graph G, which finishes the proof. $\square$

The next proposition shows that partial DFS-trees can be restricted to specific subgraphs.

Proposition 58 (Restriction of partial DFS-trees)**.** *Let T be a (partial) DFS-tree in the graph G and consider a vertex j in T which is different from the root. Denote by T' the subforest with root j obtained by restricting T to the connected component of j in the graph $G \setminus c_{T,j}$. Then T' is a (partial) DFS-tree in this same connected component.*

Proof. Observe that we only need to show that T' is connected, because the property of being a (partial) DFS-tree is, then, inherited from T. Let k be a vertex in T' different from j, we will show that the path $\overline{c}_{T,k}$ goes through j. This implies that the restriction of the path $\overline{c}_{T,k}$ to $G \setminus c_{T,j}$ provides a path between j and k in T', proving T' to be connected.

Denote by v the last common vertex of the paths $\overline{c}_{T,j}$ and $\overline{c}_{T,k}$. Observe that v is different from k because it is not in $G \setminus \overline{c}_{T,j}$. Now, if v is also different from j then two of its sons are in a same connected component of $G \setminus \overline{c}_{T,v}$, because j and k are in the same connected component of $G \setminus c_{T,j}$. But this is impossible since T is a DFS-tree. This shows that v is equal to j, and finishes the proof. □

Conversely, if T is a partial DFS-tree in the graph G, j is a leaf of T different from the root, and $\hat{T}$ is a partial DFS-tree with root j in $G \setminus (T \setminus j)$, then the rooted tree T' obtained from T by adding all edges of $\hat{T}$ is a partial DFS-tree.

Although a partial DFS-tree need not be a subtree in an intermediate step of a depth first-search algorithm, the next proposition shows that it is always a subtree of a DFS-tree.

Proposition 59. *Let T be a rooted subtree of the connected graph G. Then T is a partial DFS-tree if, and only if, it is a subtree of a DFS-tree T' with same root.*

Proof. Clearly, if T is a subtree of a DFS-tree T' with the same root, then T is a partial DFS-tree. We will prove by induction on the number of vertices of a partial DFS-tree that it is a subtree of a DFS-tree with same root. Let i be the root of the subtree T. If the partial DFS-tree T is the trivial rooted tree with the single vertex i, then one can perform a depth-first search in the connected graph G starting at i and obtain that T is a subtree of a DFS-tree T' with root i. Now, assume by induction hypothesis that T is a partial DFS-tree with more than one vertex, and that every partial DFS-tree with less vertices than T that lives in a connected graph is a subtree of a DFS-tree with same root.

Denote by $H_1, \ldots, H_k$ the connected components of $G \setminus i$. Since G is connected and T is a partial DFS-tree, one can choose for every j in $[k]$ a neighbor i_j of i in H_j, such that if H_j contains some vertex of T, then i_j is the only son of i in H_j. If i_j is a son of i in the tree T, then, by Proposition 58, the restriction T_j with root i_j of the tree T to the component H_j is a partial DFS-tree. Now, if i_j is not a son of i in the tree T, then one can define the trivial rooted tree T_j with root i_j in H_j. In any case, for every j in $[k]$, T_j is a partial DFS-tree with less vertices than T in the connected graph H_j, and so, by induction hypothesis it is a subtree of a DFS-tree T'_j with root i_j in the graph H_j.

Define T' as the spanning tree with root i of G which has exactly all of the edges $i\,i_j$ and all the edges in the trees T'_j for every j in $[k]$. Note that T is a subtree of T'. As the components $H_1, \ldots, H_k$ are disjoint and T'_j is a DFS-tree for every j, it follows that T' is a DFS-tree with root i. This proves the induction step and finishes the proof. □

The last three propositions together show that there are many (partial) DFS trees for each connected graph and give us a method for finding them.

The next result shows that DFS-trees also have an interesting property in terms of the path tree. A *maximal path* in the graph G is a path $c : i \to j$ that cannot be extended to a larger path. Notice that in this case the corresponding path in T^i_G is also maximal.

Proposition 60 (DFS-tree in a path tree)**.** *Let T be a DFS-tree with root i in the graph G. Then for every leaf j of T which is different from i, the path $\overline{c}_{T,j}$ is maximal in the graph G, and, as consequence, in the path tree T_G^i. Conversely, for every maximal path $c : i \to j$ in the connected graph G there exists a DFS-tree T with root i and leaf j such that c is equal to $\overline{c}_{T,j}$.*

Proof. If $\overline{c}_{T,j}$ is not a maximal path in the graph G, then there exists a vertex k which is not in the path $\overline{c}_{T,j}$ and such that jk is an edge in G. Since T is a DFS-tree, and the path $\overline{c}_{T,j}$ is maximal in T, there exists a vertex v, different from j and k, which is the last common point of the paths $\overline{c}_{T,j}$ and $\overline{c}_{T,k}$. But then, since jk is an edge in G, there are two sons of v in the tree T which are in the same connected component of $G \setminus \overline{c}_{T,v}$, which is impossible because T is a DFS-tree. It follows that $\overline{c}_{T,j}$ is a maximal path in the graph G.

For the second part of the statement consider a maximal path $c : i \to j$ in the connected graph G. The path c corresponds to a partial DFS-tree with root i. It follows, by Proposition 59, that there exists a DFS-tree T with root i for which c is equal to the path $\overline{c}_{T,j}$. Since c is a maximal path in G, it is also a maximal path in T, from which follows that j is a leaf of T. □

Finally, we are ready to state and prove our main result of this section, which is a new version of Sturm's theorem for graph continued fractions in terms of partial DFS-trees. Let T be a rooted subtree with root i of the graph G. Consider a time θ such that along T in the path tree T_G^i there are only plus and minus signs. In this case we can define $V_T(\theta)$ as the number of plus signs along T in T_G^i, i.e., $V_T(\theta) = |\{j \in +_{\theta,G\setminus c_{T,j}}\}_{j\in T}| = |\{j \in T \mid \alpha_j(G \setminus c_{T,j})(\theta) > 0\}|$.

Theorem 61 (Sturm's theorem for partial DFS-trees)**.** *Let T be a partial DFS-tree in the graph G. Then,*

$$\frac{\mu(G)}{\mu(G \setminus T)} = \prod_{j\in T} \alpha_j(G \setminus c_{T,j}).$$

As a consequence,

$$\sum_{x<\theta} (m_x(G) - m_x(G \setminus T)) = V_T(\theta),$$

for every real number θ, when $V_T(\theta)$ is defined.

Proof. The first part of the statement of this theorem is a reformulation of a theorem and observation by Lovász and Plummer [82, p. 338-339, Thm. 8.5.6 and Rmk. 1], and its proof is similar to Proposition 59.

We will prove by induction on the number of vertices of a partial DFS-tree that the first equality holds. Let i be the root of the partial DFS-tree T. If T is the trivial rooted tree with the single vertex i, then the equality is clearly valid. Assume, by induction hypothesis, that T is a partial DFS-tree with more than one vertex, and that the equality holds for every partial DFS-tree with less vertices than T.

Let $i_1, \ldots, i_k$ be the sons of i in the tree T. By Proposition 58, since T is partial-DFS tree, one can restrict the tree T to the partial DFS-tree T_m with root i_m in a connected component G_m of $G \setminus i$ for every m in $[k]$. Denote by G_0 the union of the components of $G\setminus i$ which are not among $G_1, \dots, G_k$, so that $G\setminus i = G_0 \sqcup G_1 \sqcup \cdots \sqcup G_k$. It follows that, $G \setminus T = G_0 \sqcup (G_1 \setminus T_1) \sqcup \cdots \sqcup (G_k \setminus T_k)$.

By induction hypothesis, since T_m is a partial DFS-tree with less vertices than T, it holds,

$$\frac{\mu(G_m)}{\mu(G_m \setminus T_m)} = \prod_{j \in T_m} \alpha_j(G_m \setminus c_{T_m,j}),$$

for every m in $[k]$. Now, as $T \setminus i = T_1 \sqcup \cdots \sqcup T_k$, it follows,

$$\alpha_j(G \setminus c_{T,j}) = \frac{\mu(G \setminus c_{T,j})}{\mu(G \setminus \bar{c}_{T,j})} = \frac{\mu(G_0) \cdots \mu(G_{m-1})\mu(G_m \setminus c_{T_m,j})\mu(G_{m+1}) \cdots \mu(G_k)}{\mu(G_0) \cdots \mu(G_{m-1})\mu(G_m \setminus \bar{c}_{T_m,j})\mu(G_{m+1}) \cdots \mu(G_k)} =$$

$$= \frac{\mu(G_m \setminus c_{T_m,j})}{\mu(G_m \setminus \bar{c}_{T_m,j})} = \alpha_j(G_m \setminus c_{T_m,j}) \implies \alpha_j(G \setminus c_{T,j}) = \alpha_j(G_m \setminus c_{T_m,j}),$$

for every j in T_m. And finally,

$$\frac{\mu(G)}{\mu(G \setminus T)} = \frac{\mu(G)}{\mu(G \setminus i)} \cdot \frac{\mu(G \setminus i)}{\mu(G \setminus T)} = \alpha_i(G) \frac{\mu(G_0)\mu(G_1) \cdots \mu(G_k)}{\mu(G_0)\mu(G_1 \setminus T_1) \cdots \mu(G_k \setminus T_k)} =$$

$$= \alpha_i(G) \prod_{m \in [k]} \frac{\mu(G_m)}{\mu(G_m \setminus T_m)} = \alpha_i(G) \prod_{m \in [k]} \prod_{j \in T_m} \alpha_j(G_j \setminus c_{T_m,j}) = \prod_{j \in T} \alpha_j(G \setminus c_{T,j}),$$

which proves the first part of the statement.

For the second part of the statement observe that, by Corollary 30, $\alpha_j(G \setminus c_{T,j})$ has only simple zeros and poles for every j in T. This fact and the first part of the statement imply that for every real number θ the number of zeros minus the number of infinities along T in T_G^i is equal to $m_\theta(G) - m_\theta(G \setminus T)$. More precisely, $|\{j \in 0_{\theta, G\setminus c_{T,j}}\}_{j \in T}| - |\{j \in \infty_{\theta, G\setminus c_{T,j}}\}_{j \in T}| = m_\theta(G) - m_\theta(G \setminus T)$, for every real number θ. This implies that the variation of the number of plus signs along T inside T_G^i at time θ is equal to $m_\theta(G) - m_\theta(G \setminus T)$. As for a large negative time all the subtrees of the path tree have negative signs, it follows that,

$$\sum_{x < \theta} m_x(G) - m_x(G \setminus T) = V_T(\theta),$$

when $V_T(\theta)$ is defined. □

Let T and T' be two partial DFS-trees in a same graph G, then the Theorem 61 implies that $\mu(G \setminus T)$ is equal to $\mu(G \setminus T')$ if, and only if, $V_T(\theta)$ is equal to $V_{T'}(\theta)$ for every time θ such that both are defined. In particular, if $G \setminus T$ and $G \setminus T'$ are isomorphic with same vertex and edge weights, then $V_T(\theta)$ is equal to $V_{T'}(\theta)$ for every θ.

Since a DFS-tree is a spanning tree, the Theorem 61 has the following corollary.

Corollary 62 (Sturm's theorem for DFS-trees)**.** *Let T be a DFS-tree in the graph G. Then, $V_T(\theta)$, when defined, is equal to the number of zeros of $\mu(G)$ in the interval $(-\infty, \theta)$.*

In particular, for every DFS-trees T and T' in a same graph G, it holds that $V_T(\theta)$ is equal to $V_{T'}(\theta)$ for every time θ such that both are defined.

Since every Hamiltonian path corresponds to a DFS-tree, the Corollary 62 is a generalization of Theorem 55. Also, in the particular case the graph is a tree the second part of Corollary 62 specializes to a result due to Godsil [51, p. 157, Thm. 7]. This also has the consequence that the total number of plus signs inside the path-tree at time θ is equal to the number of zeros of the matching polynomial of the path tree in the interval $(-\infty, \theta)$.

Note that the Corollary 62 works even if the matching polynomial does not have distinct zeros. In this case, the number of plus signs inside the DFS-tree increases not only through plus signs entering at the root of the path tree, but also with duplications inside the DFS-tree. The next example shows how this happens.

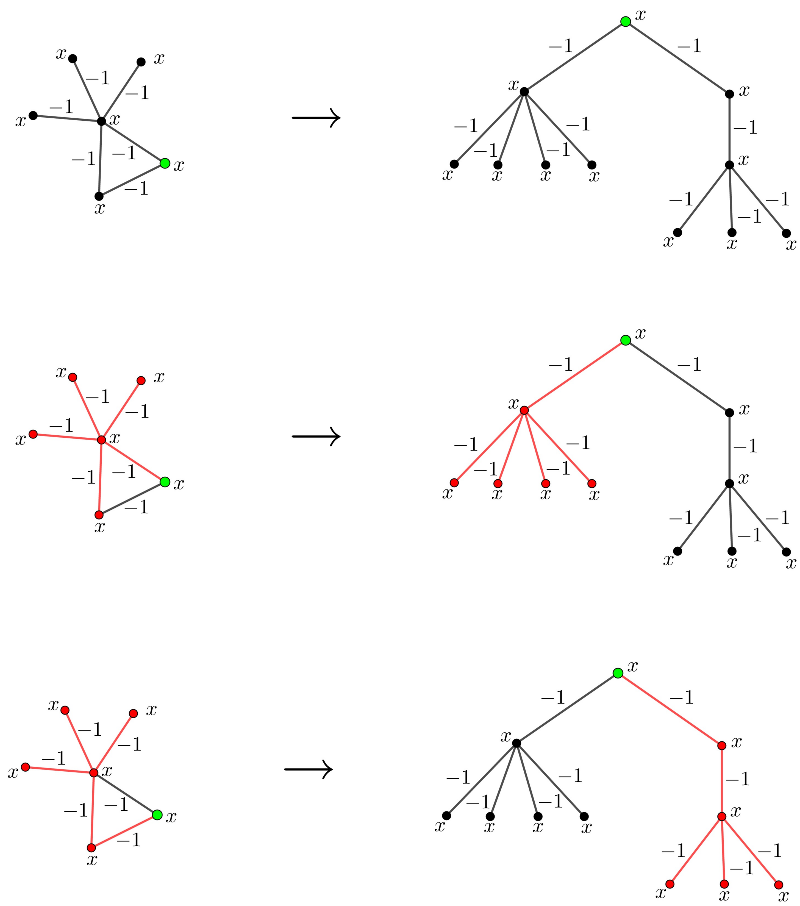


Figure 3.5: The first arrow indicates the rooted graph G and the corresponding path tree. The second and third arrows indicate in red the DFS-trees with the same root as G and their corresponding images in the path tree.

Example 63. *Consider the rooted graph G shown in Figure 3.5. This graph has the property that both spanning trees with the same root as G form DFS-trees. Observe that, by Proposition 60, the DFS-trees are made up of maximal paths, and this is seen in Figure 3.5. The matching polynomial of G is $\mu(G) = x^6 - 6x^4 + 3x^2$, and has the multi-set of zeros $\{0, 0, \pm\sqrt{3 \pm \sqrt{6}}\}$.*

In Figure 3.6 it is shown how the signs in the path-tree evolve with the time θ. Note that there is a change in some sign precisely at the zeros of the matching polynomials $\mu(G \setminus c)$, where c is a path starting at the root of G.

Observe in Figure 3.6 that the total number of plus signs at time θ along the DFS-trees in the path tree is equal to the number of zeros of $\mu(G)$ in the interval $(-\infty, \theta)$, as stated in Corollary 62. As can be seen in Figure 3.6, the number of plus signs inside the DFS-trees increases precisely at the zeros of $\mu(G)$. In particular, at time $\theta = 0$ the number of plus signs in the DFS-trees jumps from 2 to 4 because $m_0(G) = 2$, and the new plus signs come from a triplication and quadruplication.

As this last example shows, the number of plus signs along a DFS-tree can also increase by a multiplication of the plus sign inside it. Since, by Corollary 62, the number of plus signs along the DFS-tree increases at time θ by $m_\theta(G)$, the multiplication is guaranteed to happen for all DFS-trees when $m_\theta(G)$ is bigger than one.

This leads to the question of whether the Gallai-Edmonds decomposition of G at time θ can lead to the vertex of the DFS-tree for which there is a multiplication at time θ. It can be shown, using the same argument preceding the Theorem 50, that there is certainly a duplication for the vertices in $\partial 0_{\theta,G}$.

3.4 Flashes of Vertices

In order to obtain more combinatorial information from the Gallai-Edmonds decomposition, we look at the number of times that a vertex is in $0_{\theta,G}$. This is the motivation for the following definition:

Definition 64 (Flash)**.** *A vertex i of the graph G flashes at time θ if it is in $0_{\theta,G}$. The vertex i flashes k times if there are exactly k values of θ for which it is in $0_{\theta,G}$. In particular, the number of flashes of i in the graph G is equal to the number of zeros of the graph continued fraction $\alpha_i(G)$.*

The number of vertex flashes has already been considered with another name for the particular case of trees in a recent article by Johnson, Duarte and Saiago [65, p. 10], but the results for matching polynomials in this section are new.

Note that if a vertex of the graph G flashes k times then $\mu(G)$ has at least k distinct zeros. In particular if a vertex flashes the maximum possible number of times then the matching polynomial of the graph has distinct zeros. Our first result connects the number of flashes of a vertex with the length of the largest path starting at it. Recall from Section 3.3 that for a path $c : i_1 \to i_k$ we call $m_\theta(G) - m_\theta(G \setminus c)$ the *entry* (of plus signs) at time θ in the path c in $T_G^{i_1}$.

Lemma 65 (Flashes and paths)**.** *Let $c : i_1 \to i_k$ be a path in the graph G. Then c has entry equal to one at least k times. As a consequence, the vertices i_1 and i_k flash simultaneously at least k times.*

Proof. Observe that to fill in the path $c : i_1 \to i_k$ with plus signs in the path tree $T_G^{i_1}$ it must have entry equal to one in at least k times θ. By Lemma 34, for these k times θ both i_1 and i_k are simultaneously in $0_{\theta,G}$. □

This shows that vertices that are far apart flash simultaneously. Also, that the length of the largest path starting at the vertex gives a lower bound for the number of flashes. The next result, which essentially appears in the work [53, p. 12, Cor. 4.6], is a generalization of this last fact.

Proposition 66 (Flashes and largest path)**.** *Consider a path $c : i_1 \to i_k$ in the graph G and let m the number of flashes of i_k in the graph $G \setminus \{i_1, \ldots, i_{k-1}\}$. Then i_1 flashes at least $m + k - 1$ times in the graph G. In particular, if i_k flashes the maximum number of times in $G \setminus \{i_1, \ldots, i_{k-1}\}$ then i flashes the maximum number of times in G.*

Proof. Observe that at least $m-1$ plus signs must go across the path $c : i = i_1 \to i_k$ in the path tree T_G^i to get to the subtree corresponding to $\alpha_{i_k}(G \setminus \{i_1, \ldots, i_{k-1}\})$. But to fill in the path c we need an additional k plus signs. This shows that i flashes at least $m + k - 1$ times in G. □

In Section 4.3 we give another explanation for the results of Lemma 65 and Proposition 66. The next proposition shows that neighboring vertices flash at least half.

Proposition 67 (Flashes of neighbors)**.** *Let i and j be neighbors in the graph G. If i flashes m times, then j flashes at least $\left\lceil \frac{m+1}{2} \right\rceil$ times.*

Proof. Let $\theta_1, \cdots, \theta_m$ be the m times that i flashes. Observe that, by Proposition 40, the neighbor vertex j is in $0_{\theta_l,G} \sqcup \infty_{\theta_l,G}$ for every l in $[m]$. If among these m times the vertex j flashes in at least $\left\lceil \frac{m+1}{2} \right\rceil$ of them, then the result follows. For this reason, assume that j is in $\infty_{\theta_l,G}$ for at least $\left\lfloor \frac{m}{2} \right\rfloor$ values of l in $[m]$. Now notice that the number of times for which a vertex is in $\infty_{\theta,G}$ is one less than the total number of its flashes. This implies that j flashes at least $\left\lfloor \frac{m}{2} \right\rfloor + 1$ times, which finishes the proof. □

The statement of Proposition 67 can be seen as the analogue of the following fact for largest paths: Let i and j be neighbors in the graph G. If the length of the largest path starting at i is m, then the length of the largest path starting at j is at least $\left\lceil \frac{m+1}{2} \right\rceil$. The reason for this analogy will become more clear in Section 4.3. Also note that the bound in Proposition 67 is sharp, as can be seen in the example of Figure 3.7.

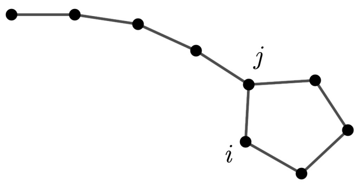


Figure 3.7: Neighboring vertices i and j flash 9 and 5 times, respectively.

The next result uses the rooted product of graphs defined in Section 2.3.

Proposition 68 (Rooted product of graphs)**.** *Let i and j be vertices in the graphs G and H, respectively. Consider the rooted product $G \circ_j H$ of G and H where the root of H is the vertex j. Then the following relation holds,*

$$\alpha_i(G \circ_j H) = \alpha_i(G) \circ \alpha_j(H).$$

Proof. This is an immediate consequence of Lemma 23. □

Corollary 69 (Multiplication of flashes)**.** *If i flashes l times in the graph G and j flashes m times in the graph H, then i flashes $l \cdot m$ times in the graph $G \circ_j H$. In particular, if i and j are maximum flashers in the graphs G and H respectively, then i is a maximum flasher in the graph $G \circ_j H$.*

Proof. Observe that the number of flashes is equal to the number of branches of a graph continued fraction. Thus $\alpha_i(G)$ and $\alpha_j(H)$ have l and m branches, respectively, which implies that the composition $\alpha_i(G) \circ \alpha_j(H)$ has $l \cdot m$ branches. But from Proposition 68 it holds $\alpha_i(G \circ_j H) = \alpha_i(G) \circ \alpha_j(H)$, and as a consequence the graph continued fraction $\alpha_i(G \circ_j H)$ has $l \cdot m$ branches. This shows that i flashes $l \cdot m$ times in $G \circ_j H$. □

The next example shows that although the number of flashes and length of the largest path have a connection, the former may be much larger than the later.

Example 70. *Let G be the graph with vertex set $[2]$ where there is an edge between the two vertices. Assume that vertices weights is x and the edge weight is -1. Note that the graph continued fraction for any of the vertices is $x - \dfrac{1}{x}$. This implies that both vertices of G are maximum flashers.*

Consider now the sequence of graphs $(G_n)_{n \geq 1}$, where $G_1 = G$ and $G_{n+1} = G_n \circ_1 G$ for every n bigger than, or equal to, one. Observe that G_n is a tree with 2^n vertices and the length of its largest path is $2n-1$. Now, since G has only maximum flashers, this implies, by Corollary 69, that G_n has a maximum flasher for every n. Closer analysis actually shows that all vertices of G_n are maximum flashers for every n.

It follows that for every natural number n the graph G_n has a vertex that flashes 2^n times while the length of its largest path is $2n-1$. This shows that the number of flashes of a vertex may be much larger than the length of the largest path starting at it.

In the next chapter we present some other connections between the number of flashes and paths using combinatorial formulas for graph continued fractions.

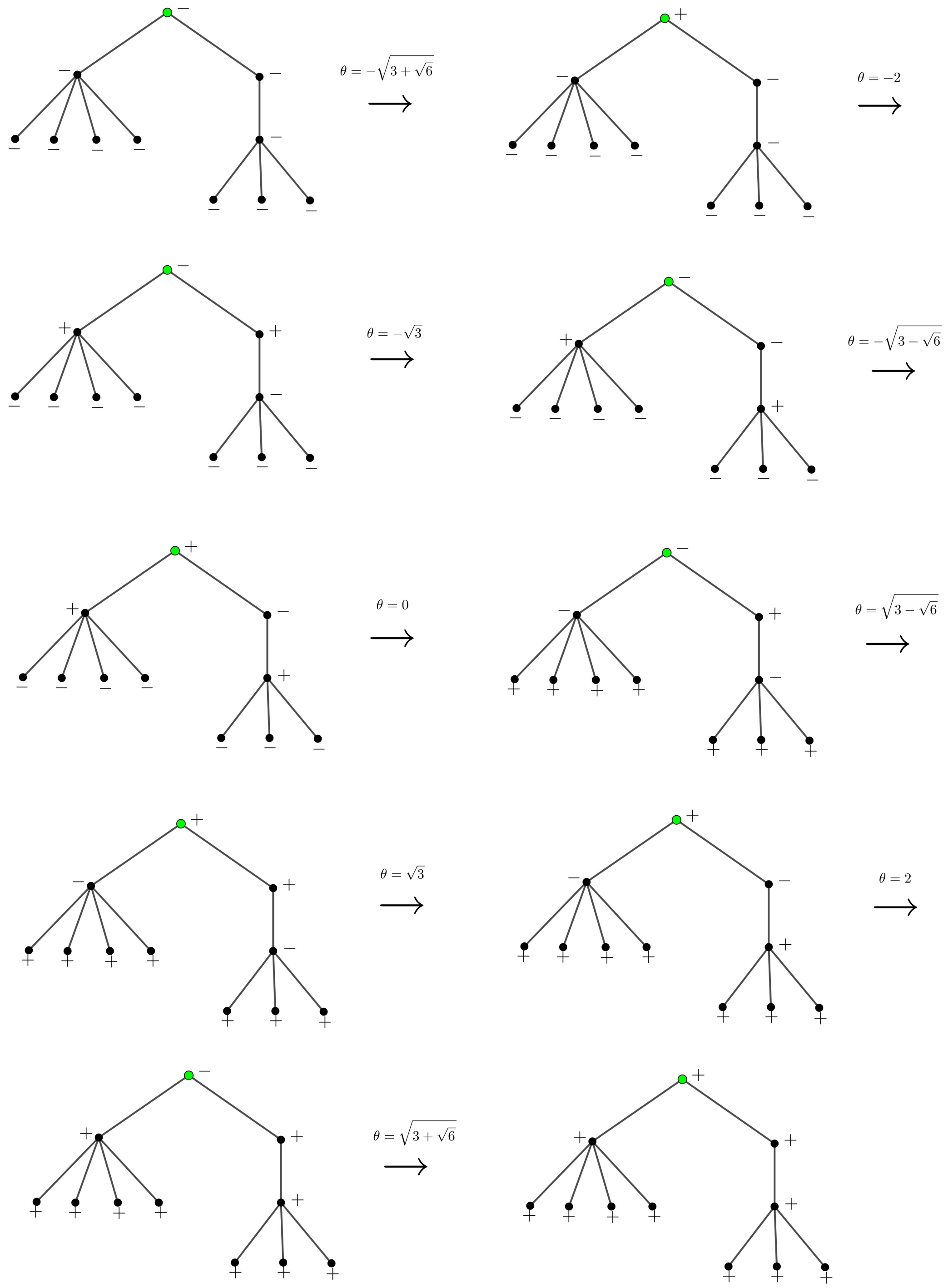


Figure 3.6: The signs are from the subtrees of the path tree of G shown in Figure 3.5. As time passes the plus signs fill in the path tree of the graph G.

Chapter 4

Combinatorial Formulas

In this chapter, we begin by recalling in Section 4.1 some basic facts and formulas of the classical theory of orthogonal polynomials. Next, in Section 4.2 we pay special attention to this theory in a discrete setting involving interlacing polynomials. In Section 4.3, inspired by the theorems of the theory of orthogonal polynomials, we present some parallel results between spectral properties of characteristic and matching polynomials.

In Section 4.3.1 we characterize the number of distinct zeros of a matching polynomial in terms of the dimension of a vector space generated by the matching polynomials of a family of subgraphs and prove analogous result for characteristic polynomials in terms of the adjugate matrix.

In Section 4.3.2 we present some formulas for quotients of characteristic polynomials and graph continued fractions that allow us to recover some classic results of the theory of distance regular graphs and prove analogous results to matching polynomials. In particular, we prove that the sub-discriminants of characteristic and matching polynomials can be written as a sum of squares, and we present an upper bound for the number of paths starting at some vertex i of a graph G using only the matching polynomials of G and $G \setminus i$.

Finally, in Section 4.3.3, we show that the formulas in Section 4.3.2 generalize to locally-finite graphs and we prove an upper bound for the connective constant of a locally-finite vertex-transitive graph in terms of matchings.

4.1 Orthogonal Polynomials

In this section, we recall some basic facts about the classical theory of orthogonal polynomials [24, 69, 100]. We focus on the equations satisfied by the various objects, and in the next section pay special attention to the discrete version of the theory, which is connected to graph continued fractions and interlacing polynomials.

Let τ be a measure in $\mathbb{R}$ with finite moments, i.e., $\tau_n := \displaystyle\int_{\mathbb{R}} r^n d\tau(r)$ is finite for every n in $\mathbb{N} \cup \{0\}$, and consider the associated linear map $\mathcal{L} : \mathbb{R}[x] \to \mathbb{R}$,

$\mathcal{L}(p) := \int_{\mathbb{R}} p(r)d\tau(r)$. This map comes equipped with the scalar product given by $< p, q >:= \mathcal{L}(pq)$. The *orthogonal polynomial sequence* associated with τ is the unique sequence of monic orthogonal polynomials with respect to this scalar product. This sequence is finite if, and only if, the measure τ consists of a finite number of atoms.

Denote by $(p_n(x))_{n\geq 0}$ the orthogonal polynomial sequence associated with the measure τ, where $\deg p_n = n$ for every n in $\mathbb{N}\cup\{0\}$. It is a classical result [24, p. 18, Thm. 4.1] that the sequence $(p_n(x))_{n\geq 0}$ satisfies a three term recurrence:

$$p_{n+1}(x) = (x - r_{n+1})p_n(x) + \lambda_n p_{n-1}(x),\ \forall n \in \mathbb{N},$$

where r_n is a real number and λ_n is negative for every natural number n. Conversely, a classical theorem of Favard [38] (or see [24, p. 21, Thm. 4.4]) states that every sequence of monic polynomials that satisfies a three term recurrence of this type is an orthogonal polynomial sequence for some measure in $\mathbb{R}$ with finite moments.

In general there can be more than one measure with the same orthogonal polynomial sequence. The classical *moment problem* consists in determining conditions under which an orthogonal polynomial sequence is associated with a unique measure. A well-known solution to the moment problem that interests us, and that will be useful later, is that whenever both sequences $(r_n)_{n\geq 0}$ and $(\lambda_n)_{n\geq 0}$ are bounded, the measure associated with the orthogonal polynomial sequence is unique and has bounded support.

In this thesis we are particularly interested in simple equations connecting the measure τ, the moments τ_n and the three term recurrence coefficients that the orthogonal polynomial sequence satisfies. The fundamental equation connecting these objects comes from the *Stieltjes transform* of the measure τ:

$$\int_{\mathbb{R}} \frac{d\tau(r)}{x-r} = \sum_{n\geq 0} \frac{\tau_n}{x^{n+1}} = \cfrac{\tau_0}{x - r_1 + \cfrac{\lambda_1}{x - r_2 + \cfrac{\lambda_2}{x - r_3 + \cdots}}}.$$

Observe that the negative of the Stieltjes transform of τ is a function $f(x)$ from the upper half-plane to itself. In this sense, the last equation can be interpreted as showing three ways of writing this special function $f(x)$: as the negative of a Stieltjes transform, a Laurent series at infinity and as a continued fraction. From this point of view, the moment problem is to determine to what extent the representation of the function $f(x)$ as the negative of a Stieltjes transform is unique.

It is also clear that the Laurent series for $f(x)$ is always unique and that the continued fraction can be obtained from the Laurent series by means of a continued fraction algorithm. This simple algorithm is presented in Khrushchev's book [69, p. 250, Thm. 6.2]. In addition to its use in orthogonal polynomial theory, such an algorithm is the main ingredient for the Berlekamp-Massey algorithm [103] in error-correction codes theory, which serves to determine the minimal polynomial of a linear recurrent sequence in an arbitrary field.

It was already known to Sylvester [99, p. 474], at least if the measure τ consists of a finite number of atoms, as the measure τ, moments, three term recurrence coefficients and orthogonal polynomial sequence are more directly related:

$$\Delta_n := \frac{1}{n!}\int_{\mathbb{R}^n} \prod_{\{j,k\}\subseteq[n]} (x_j - x_k)^2 d\tau(x_1)\cdots d\tau(x_n) = \det\begin{bmatrix} \tau_0 & \tau_1 & \tau_2 & \cdots & \tau_{n-1} \\ \tau_1 & \tau_2 & \ddots & \ddots & \tau_n \\ \tau_2 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \tau_{n-1} & \tau_n & \cdots & \cdots & \tau_{2n-2} \end{bmatrix} =$$

$$= (-1)^{\frac{n(n-1)}{2}} \tau_0^n \lambda_1^{n-1} \lambda_2^{n-2} \cdots \lambda_{n-1}^1,$$

and also,

$$\chi_n := \frac{1}{n!}\int_{\mathbb{R}^n} (x_1 + \cdots + x_n) \prod_{\{j,k\}\subseteq[n]} (x_j - x_k)^2 d\tau(x_1)\cdots d\tau(x_n) =$$

$$= \det\begin{bmatrix} \tau_0 & \tau_1 & \cdots & \tau_{n-2} & \tau_{n-1} \\ \tau_1 & \tau_2 & \cdots & \tau_{n-1} & \tau_n \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \tau_{n-2} & \tau_{n-1} & \cdots & \tau_{2n-4} & \tau_{2n-3} \\ \tau_n & \tau_{n+1} & \cdots & \tau_{2n-2} & \tau_{2n-1} \end{bmatrix} = (r_1 + \cdots + r_n)\Delta_n,$$

$$\frac{1}{\Delta_{n+1}\Delta_n}\int_{\mathbb{R}} x \left(\frac{1}{n!}\int_{\mathbb{R}^n} \prod_{j\in[n]} (x - x_j) \prod_{j<k\leq n} (x_j - x_k)^2 d\tau(x_1)\cdots d\tau(x_n) \right)^2 d\tau(x) =$$

$$= \frac{\chi_{n+1}}{\Delta_{n+1}} - \frac{\chi_n}{\Delta_n} = r_{n+1},$$

and,

$$p_n(x) = \frac{1}{\Delta_n n!}\int_{\mathbb{R}^n} \prod_{j\in[n]} (x - x_j) \prod_{j<k\leq n} (x_j - x_k)^2 d\tau(x_1)\cdots d\tau(x_n) =$$

$$= \frac{1}{\Delta_n}\det\begin{bmatrix} \tau_0 & \tau_1 & \tau_2 & \cdots & \tau_n \\ \tau_1 & \tau_2 & \ddots & \ddots & \tau_{n+1} \\ \tau_2 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \tau_{n-1} & \tau_n & \cdots & \cdots & \tau_{2n-1} \\ 1 & x & x^2 & \cdots & x^n \end{bmatrix},$$

for every natural number n.

In Section 4.3 it will be shown that generalizations of these formulas are valid for graph continued fractions and admit combinatorial interpretations.

There are also direct formulas connecting the orthogonal polynomial sequence, measure, moments and linear map. In a recent paper, Garsia and Ganzberger [47] explain these formulas for orthogonal polynomials using Viennot's Heaps of Pieces theory [101].

The next three theorems are simple examples of the connection between the measure τ and the zeros of the orthogonal polynomial sequence. These classical results are present in Chihara's book [24].

Theorem 71 ([24], p. 27, Thm. 5.2)**.** *Let τ be a measure in $\mathbb{R}$ with finite moments and orthogonal polynomial sequence $(p_n(x))_{n\geq 0}$ and consider a closed interval I that contains the support of τ. Then the zeros of $p_n(x)$ are all real, simple and located in the interior of I.*

Theorem 72 (Gauss quadrature formula [24], p. 32, Thm. 6.1)**.** *Consider a measure τ in $\mathbb{R}$ with finite moments and let $x_1^n < \cdots < x_n^n$ be the zeros of $p_n(x)$ for some natural number n. Then there are positive numbers $a_1^n, \ldots, a_n^n$ such that for every polynomial $\rho(x)$ of degree at most $2n-1$ it holds,*

$$\mathcal{L}(\rho) = \int_{\mathbb{R}} \rho(r) d\tau(r) = \sum_{j\in[n]} a_j^n \rho(x_j^n).$$

Theorem 73 (Interlacing for orthogonal polynomials [24], p. 34, Thm. 6.2)**.** *Let $(p_n(x))_{n\geq 0}$ be an orthogonal polynomial sequence. Then, between any two zeros of $p_m(x)$ there is a zero of $p_n(x)$ for every $n > m \geq 2$.*

Proof. Let a and b be two consecutive zeros of $p_n(x)$ and assume, by contradiction, that the polynomial $p_m(x)$, with m bigger than n, does not have a zero in $[a, b]$. Now, $\rho(x) := \dfrac{p_m(x)}{(x-a)(x-b)}$ is a polynomial of degree $m-2$ and $\rho(x)p_m(x) \geq 0$ for every x not in (a, b). Since $p_n(x)$ does not have zeros in (a, b) it follows by Theorem 72 that,

$$< \rho, p_m >= \mathcal{L}(\rho p_m) = \sum_{j\in[n]} a_j^n \rho(x_j^n) p_m(x_j^n) > 0.$$

But the polynomial $\rho(x)$ has degree $m-2$ and so it can be written as a linear combination $\rho(x) = \sum_{j=0}^{m-2} b_j p_j(x)$, from which follows $< \rho, p_m >= 0$, reaching a contradiction. $\square$

Since by Favard's theorem [38] the orthogonal polynomial sequences are precisely the sequences of polynomials that satisfy a three term recurrence, the interlacing of the Theorem 73 is true for every sequence of polynomials satisfying a three term recurrence.

As will be seen in the next section, interlacing polynomials can be used as the starting point for the theory of orthogonal polynomials for discrete measures.

4.2 Interlacing Polynomials and Sturm Sequences

In this section, we consider orthogonal polynomials for a measure with a finite number of atoms. It will be convenient to start with two interlacing polynomials.

Consider two real monic polynomials p and q of degrees n and $n-1$, respectively, with real, distinct and interlaced zeros. We are interested in ways to write the quotient $\dfrac{p}{q}(x)$ and how to get from one to another.

The quotient $\dfrac{p}{q}(x)$ can be written as:

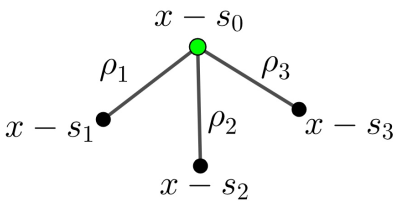
$$\frac{p}{q}(x) = x - s_0 + \sum_{j=1}^{n-1} \frac{\rho_j}{x - s_j} = x - s_0 + \sum_{n \geq 0} \frac{\tau_j}{x^{n+1}} = x - s_0 + \cfrac{\lambda_1}{x - r_1 + \cfrac{\lambda_2}{\ddots + \cfrac{\lambda_{n-1}}{x - r_{n-1}}}},$$

where ρ_j and λ_j are negative and s_j, τ_j and r_j are real for every j. Note that the last two equalities appear in the previous section and the last equality also appears in the beggining of Section 3.3. The observation that the coefficients in the partial fraction and continued fraction are negative is due to Sylvester [99, p. 474], but this fact also follows from the theory presented in the previous section. As mentioned in Section 3.3 the sequence of partial numerators of the continued fraction is known as the Sturm sequence for the pair $(p(x), q(x))$ and is the initial segment of an orthogonal polynomial sequence.

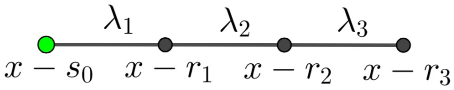
It is also interesting to note that the functions $\pm\dfrac{p}{q}$ appear in ergodic theory [80, p.277], since they are precisely the rational functions of $\mathbb{R}(x)$ that preserve the Lebesgue measure in $\mathbb{R}$.

We call canonical forms the following four different ways of writing the quotient $\dfrac{p}{q}(x)$: as it is; as a partial fraction; as a Laurent series; as a continued fraction. Observe that both the partial fraction and continued fraction expansions of $\dfrac{p}{q}(x)$ can be written as a graph continued fraction of a star and a path graphs, respectively. In Figure 4.1 we show an example of these two representations. For this reason, we refer to these two canonical forms as *star continued fraction* and *path continued fraction*. The number of vertices in both the star and path continued fractions of the quotient $\dfrac{p}{q}(x)$ is equal to the number of zeros of $\dfrac{p}{q}(x)$.

Similarly, one can write the inverse $\dfrac{q}{p}(x)$ as a partial fraction, Laurent series and continued fraction and talk about its canonical forms. In this case, new coefficients and information are obtained that do not appear in the canonical forms of $\dfrac{p}{q}(x)$ (with the exception of the continued fraction coefficients which are equal). Also note that in this case the theory is closer to that presented in Section 4.1. However, we mainly use the canonical forms of the quotient $\dfrac{p}{q}(x)$, because of the connection to graph continued fractions.



$$= \quad x - s_0 + \frac{\rho_1}{x - s_1} + \frac{\rho_2}{x - s_2} + \frac{\rho_3}{x - s_3}$$



$$= \quad x - s_0 + \cfrac{\lambda_1}{x - r_1 + \cfrac{\lambda_2}{x - r_2 + \cfrac{\lambda_3}{x - r_3}}}$$

Figure 4.1: In the first part, there is a representation of a partial fraction expansion as the graph continued fraction of a star. In the second part, there is the representation of a continued fraction as the graph continued fraction of a path.

A natural question is how to move from one canonical form to another. Consider the case where the polynomials p and q are given in terms of their coefficients. In this case, it is clearly possible to obtain a closed formula from one canonical form to another, with the exception that there is no closed formula for a star continued fraction. This exception occurs because there is no general formula a polynomial's zeros in terms of their coefficients. Such expressions for moving between canonical forms can be obtained directly from the definition and formulas presented in the previous section.

If there is not a simple closed formula from one canonical form to another, the next best thing to want is an easy algorithm. For example, to obtain the path continued fraction from the quotient, just run the Euclidean algorithm for $\frac{p}{q}(x)$.

For each family of interlacing polynomials originating from a combinatorial object, it is expected that there is a combinatorial interpretation for its canonical forms. Note that the edge coefficients of the path continued fraction are always computable and negative, which not only suggests that they count something, but also that they may be written as the negative of a sum of squares. These coefficients can be studied for small cases using some mathematical software, e.g. Sage or Mathematica.

Both characteristic and matching polynomials satisfy interlacing by Corollaries 6 and 31, respectively. This raises the question of what the combinatorial interpretations of canonical forms are in these two cases. Note that for Laurent series there is already a combinatorial interpretation in terms of walks and tree-like walks by the Theorems 7 and 24. The question now is whether anything significant can be said about the star and path continued fractions representations. This will be the topic of the next section.

4.3 Graph Continued Fraction to Canonical Forms

In this section, we establish the star and path continued fractions for quotients of characteristic polynomials and graph continued fractions. We show how the star continued fraction leads to a relationship between distinct zeros of matching polynomials and linear independence of matching polynomials of subgraphs. We also show how the path continued fraction naturally leads to bounds for paths that start at the root of the graph continued fraction.

4.3.1 Star Continued Fraction

Although there is no closed formula for the star continued fraction of a quotient of characteristic polynomials, there is an interpretation for the inverted quotient in terms of eigenvectors of the adjacency matrix.

Let $\{v_1, \cdots, v_n\}$ be an orthonormal eigenbasis for the hermitian matrix $-A_G(0)$. For an eigenvalue θ of $-A_G(0)$, i.e., a zero of the characteristic polynomial $\phi(G)$, denote by S_θ the set of indexes of the eigenvectors associated with θ. Recall that $adj(B)$ denotes the adjugate of the matrix B.

Theorem 74 (Godsil [52], p. 27-30)**.** *For every graph G it holds,*

$$\frac{adj(A_G(x))}{\phi(G)(x)} = \sum_{\phi(G)(\theta)=0} \frac{\sum_{k\in S_\theta} v_k v_k^T}{x-\theta}.$$

The sum $\sum_{k\in S_\theta} v_k v_k^T$ is independent of the initial choice of orthonormal eigenbasis $\{v_1, \dots, v_n\}$ and the multiplicity of θ as a zero of $\phi(G)$ is equal to the rank of $\sum_{k\in S_\theta} v_k v_k^T$, for every θ that is a zero of $\phi(G)$.

As a corollary of this last theorem, there is the following partial fraction expansion for the adjugate matrix entries.

Corollary 75. *For every graph G and vertices i and j it holds,*

$$\frac{(adj(A_G(x)))_{i,j}}{\phi(G)(x)} = \sum_{\phi(G)(\theta)=0} \frac{\sum_{k\in S_\theta} (v_k)_i (v_k)_j}{x-\theta}.$$

In particular,

$$\frac{\phi(G\setminus i)}{\phi(G)}(x) = \frac{(adj(A_G(x)))_{i,i}}{\phi(G)(x)} = \sum_{\phi(G)(\theta)=0} \frac{\sum_{k\in S_\theta} (v_k)_i^2}{x-\theta}.$$

As observed by Godsil [52, p. 29, Thm. 5.3] this last result implies Cauchy's interlacing for characteristic polynomials, which is described in Corollary 6 of this work. The Corollary 75 also appears in the work of Van Mieghem [86, p. 6, Cor. 2], where it is used in the study of a centrality metric for graphs. A reformulation of the second equation in Corollary 75 has recently received a lot of attention as explained in the article [29].

We now show how Corollary 75 gives a relationship between zeros of $\phi(G)$ and the vector spaces of polynomials generated by entries of the adjugate matrix $adj(A_G(x))$. Given a vertex i in the graph G denote by V_G and V_G^i the vector spaces of polynomials generated by $\{(adj(A_G(x)))_{jk}\}_{j,k\in[n]}$ and $\{(adj(A_G(x)))_{i,j}\}_{j\in[n]}$, respectively. Note that $V_G = \sum_{i\in[n]} V_G^i$. Also, denote by H_G^i the set of zeros of $\dfrac{\phi(G)}{\phi(G\setminus i)}$.

Theorem 76. *For every graph G it holds that:*

a) The number of distinct zeros of $\phi(G)$ is equal to the dimension of V_G;

b) The number of zeros of $\dfrac{\phi(G)}{\phi(G\setminus i)}$ is equal to the dimension of V_G^i;

c) The cardinality of every finite expression obtained from $\{H_G^i\}_{i\in[n]}$ using intersections and unions is equal to the dimension of the same expression where each H_G^i is replaced by V_G^i and the unions are replaced by sums.

Proof. a) This item is a consequence of the item (c). The following equation is from Lemma 8:

$$\frac{\phi(G)'}{\phi(G)}(x) = \sum_{i\in[n]} \frac{\phi(G\setminus i)}{\phi(G)}(x).$$

This equation implies that θ is a zero of $\phi(G)$ if, and only if, it is among the zeros of $\dfrac{\phi(G)}{\phi(G\setminus 1)}, \ldots, \dfrac{\phi(G)}{\phi(G\setminus n)}$. From this it follows by the item (c) that the number of zeros of $\phi(G)$ is equal to $|H_G^1 \cup \cdots \cup H_G^n| = \dim V_G^1 + \cdots + V_G^n = \dim V_G$, as we wanted.

b) We need to show that the number of poles of $\dfrac{\phi(G\setminus i)}{\phi(G)}$ is equal to the dimension of V_G^i. To do this we prove a more precise statement from which both this result and item (c) follow. If $\phi(G)$ has m distinct zeros $\theta_1, \ldots, \theta_m$, then the vector space V_G^i can be identified with the vector space generated by,

$$\left\{ \left(\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_j, \ldots, \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_j \right) \right\}_{j\in[n]}.$$

To prove this, first notice that by Corollary 75,

$$
\begin{bmatrix}
\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_1 & \cdots & \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_1 \\
\vdots & \ddots & \vdots \\
\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_n & \cdots & \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_n
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{|S_{\theta_1}|}{x_1-\theta_1} & \cdots & \frac{|S_{\theta_1}|}{x_m-\theta_1} \\
\vdots & \ddots & \vdots \\
\frac{|S_{\theta_m}|}{x_1-\theta_m} & \cdots & \frac{|S_{\theta_m}|}{x_m-\theta_m}
\end{bmatrix}
=
$$

$$
= \begin{bmatrix}
(adj(A_G(x_1)))_{i1} & \cdots & (adj(A_G(x_m)))_{i1} \\
\vdots & \ddots & \vdots \\
(adj(A_G(x_1)))_{in} & \cdots & (adj(A_G(x_m)))_{in}
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{1}{\phi(G)(x_1)} & 0 & \cdots & 0 \\
0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & \frac{1}{\phi(G)(x_m)}
\end{bmatrix},
$$

for every $x_1 \ldots, x_m$ which are distinct and different from $\theta_1, \ldots, \theta_m$. Observe that the second matrix in this last equation is invertible, since its determinant can be evaluated to,

$$
\det \begin{bmatrix}
\frac{|S_{\theta_1}|}{x_1-\theta_1} & \cdots & \frac{|S_{\theta_1}|}{x_m-\theta_1} \\
\vdots & \ddots & \vdots \\
\frac{|S_{\theta_m}|}{x_1-\theta_m} & \cdots & \frac{|S_{\theta_m}|}{x_m-\theta_m}
\end{bmatrix}
= |S_{\theta_1}| \cdots |S_{\theta_m}| \frac{\prod_{\{j,k\}\subseteq[m]} (x_j - x_k)(\theta_k - \theta_j)}{\prod_{j,k\in[m]} (x_j - \theta_k)},
$$

using *Cauchy's double alternant* [70, p. 355, Eq. 2.7]. Since $x_1, \ldots, x_m$ are not zeros of $\phi(G)$, the diagonal matrix in the equation above is also invertible. Now, since the only condition on $x_1, \ldots, x_m$ is that they are distinct, one can use a vandermonde matrix argument to conclude that the vector space V_G^i can be identified with,

$$
\left\{ \left(\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_j, \ldots, \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_j \right) \right\}_{j\in[n]}.
$$

Now, notice that,

$$
\begin{bmatrix}
\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_1 & \cdots & \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_1 \\
\vdots & \ddots & \vdots \\
\sum_{k\in S_{\theta_1}} (v_k)_i (v_k)_n & \cdots & \sum_{k\in S_{\theta_m}} (v_k)_i (v_k)_n
\end{bmatrix}
=
\begin{bmatrix}
(v_1)_1 & \cdots & (v_n)_1 \\
\vdots & \ddots & \vdots \\
(v_1)_n & \cdots & (v_n)_n
\end{bmatrix}
\cdot B_i,
$$

where B_i is the $n \times m$ matrix with entry $(B_i)_{kl}$ equal to $(v_k)_i$, if k is in S_{θ_l}, or 0, otherwise, for every k in $[n]$ and l in $[m]$. Since the second matrix in this last equation is invertible, because $\{v_1, \ldots, v_n\}$ is linear independent, this implies that V_G^i can be identified with the subspace U_i of R^m generated by the rows of the matrix B_i. Observe that the l-th column of B_i is different from zero if, and only if, $\sum_{k \in S_{\theta_l}} (v_k)_i^2 \neq 0$. Since $[n]$ is the disjoint union of $S_{\theta_1}, \ldots, S_{\theta_m}$ it follows, by the definition of B_i, that a set of rows of B_i is linear independent if, and only if, no two indexes of these rows are in a same S_{θ_l} for some l in $[m]$. Putting it all together, it follows that,

$$U_i = \left\{ (x_1, \ldots, x_m) \in \mathbb{R}^m \,\middle|\, x_l = 0 \text{ for every } l \text{ s.t. } \sum_{k \in S_{\theta_l}} (v_k)_i^2 = 0 \right\}.$$

Finally, observe that, by Corollary 75, θ_l is a pole of $\dfrac{\phi(G \setminus i)}{\phi(G)}$ if, and only if, $\sum_{k \in S_{\theta_l}} (v_k)_i^2 \neq 0$. It follows that the dimension of V_G^i, which is the same as the dimension of U_i, is equal to the number of poles of $\dfrac{\phi(G \setminus i)}{\phi(G)}$, proving item (b).

$c)$ Observe that in the last part of the proof of item (b) there is characterization of H_G^i in terms of the non-zero coordinates of vectors in U_i. Using this characterization, it follows that the cardinality of every finite expression obtained from $\{H_G^i\}_{i \in [n]}$ using intersections and unions is equal to the dimension of the same expression where each H_G^i is replaced by U_i and the unions are replaced by sums. Finally, since for every i the space U_i is in correspondence with the space V_G^i through a same linear transformation, the result follows. $\square$

The item (a) of Corollary 76 is generally stated in terms of the *walk matrix* of a graph and appears in Hagos' work [63, p. 104, Thm. 2.1]. Item (b) of Corollary appears in Godsil's article [54, p. 886, Cor. 7.2] in terms of the walk matrix.

In the particular case that the graph is a tree T, the adjugate matrix $adj(A_T(x))$ has a nice form. Given vertices i and j of T denote by $i \to j$ the unique path from i to j.

Theorem 77 (Godsil [51], p. 156, Thm. 6)**.** *Let i and j be vertices in the tree T. Then,*

$$(adj(A_T(x)))_{i,j} = \rho_{i \to j} \phi(T \setminus i \to j)(x).$$

The Theorems 76 and 77 together imply an interpretation for the number of flashes of a vertex in terms of vector spaces of matching polynomials of subgraphs.

For a vertex i in the graph G we denote by $[i \to \cdot]$ the set of paths starting at i, and write $[\cdot \to \cdot]$ for the set of paths in the graph G, when there is no danger of confusion. Given two distinct vertices i and j in the graph G denote by W_G, W_G^i and $W_G^{i,j}$ the vector spaces of polynomials generated by $\{\mu(G \setminus c)\}_{c \in [\cdot \to \cdot]}$, $\{\mu(G \setminus c)\}_{c \in [i \to \cdot]}$ and $\{\mu(G \setminus c)\}_{c \in [i \to j]}$, respectively. Observe that $W_G = \sum_{i \in [n]} W_G^i$ and $W_G^i = \sum_{j \in [n]} W_G^{i,j}$.

Also, denote by F_G^i the set of times θ such that i flashes. Note that by Lemma 32 the set of zeros of $\mu(G)$ is precisely $\bigcup_{i\in[n]} F_G^i$.

In this case, there is our new analogous statement of Theorem 76 for matching polynomials.

Theorem 78. *For every graph G it holds that:*

a) The number of distinct zeros of $\mu(G)$ is equal to the dimension of W_G;

b) The number of flashes of i is equal to the dimension of W_G^i;

c) The cardinality of every finite expression obtained from $\{F_G^i\}_{i\in[n]}$ using intersections and unions is equal to the dimension of the same expression where each F_G^i is replaced by W_G^i and the unions are replaced by sums.

Proof. $a)$ Since the set of zeros of $\mu(G)$ is equal to $\bigcup_{i\in[n]} F_G^i$ this result follows from item (c).

$b)$ By Godsil's Lemma 16 it holds $\alpha_i(G) = \dfrac{\mu(T_G^i)}{\mu(T_G^i \setminus i)} = \dfrac{\phi(T_G^i)}{\phi(T_G^i \setminus i)}$. This implies that the number of flashes of i is equal to the number of zeros of $\dfrac{\phi(T_G^i)}{\phi(T_G^i \setminus i)}$. By Theorem 76 this number of zeros is equal to the dimension of the vector space $V_{T_G^i}^i$, which is generated by the polynomials $\{(adj(A_{T_G^i}(x)))_{i,j} | \ j$ is a vertex of $T_G^i\}$. Since T_G^i is a tree, the Theorem 77 implies that $(adj(A_{T_G^i}(x)))_{i,j} = \rho_{i\to j}\phi(T_G^i \setminus i \to j)(x)$ for every vertex j of T_G^i. It follows that the dimension of $V_{T_G^i}^i$ is equal to the dimension of the vector space generated by $\{\phi(T_G^i \setminus c)\}_{c\in[i\to\cdot]}$.

Recall that, by the definition of path tree, the paths of G in $[i \to \cdot]$ are in direct correspondence with the paths of T_G^i in $[i \to \cdot]$. This fact together with Godsil's Lemma 16 implies that for every path c of T_G^i in $[i \to \cdot]$ it holds,

$$\frac{\phi(T_G^i \setminus c)}{\phi(T_G^i)} = \frac{\mu(T_G^i \setminus c)}{\mu(T_G^i)} = \frac{\mu(G \setminus c)}{\mu(G)}.$$

As a consequence, the dimension of the vector space generated by $\{\phi(T_G^i \setminus c)\}_{c\in[i\to\cdot]}$ is equal to the dimension of the vector space W_G^i generated by $\{\mu(G \setminus c)\}_{c\in[i\to\cdot]}$. This proves that the number of flashes of i is equal to the dimension of W_G^i.

$c)$ Observe that, unlike in the proof of item (b), one cannot directly apply the Theorem 76 to prove this item, because for distinct vertices i and j of the graph G the path trees T_G^i and T_G^j are not isomorphic in general. However, for every vertex i of G one can consider the vector space U_i associated with the poles of $\dfrac{\phi(T_G^i \setminus i)}{\phi(T_G^i)}$ as given in the proof of the item (b) of Theorem 76. Since by Godsil's Lemma 16 it holds $\dfrac{\phi(T_G^i \setminus i)}{\phi(T_G^i)} = \dfrac{\mu(G \setminus i)}{\mu(G)}$ for every vertex i, one can see that all the vector spaces U_i obtained this way can be considered inside of a same space $\mathbb{R}^m$ where m is the number of distinct zeros of $\mu(G)$. Using this observation the proof is analogous to that of item (c) of Theorem 76. $\square$

The Theorem 78 provides a refinement of the result by Godsil [50, p. 296, Cor. 5.3] that the matching polynomial of a graph with a path of length l has at least $l+1$ distinct zeros. It is easy to see that Theorem 78 implies this result. Indeed, if G has a path $c : i_1 \to i_{l+1}$ and c_j denotes sub-path from i_1 to i_j for every j in $[l+1]$, then $\{\mu(G \setminus c_j)\}_{j \in [l+1]}$ has dimension $l+1$, since the degree of $\mu(G \setminus c_j)$ is equal to the degree of $\mu(G)$ minus j for every j in $[l+1]$. This shows that the dimension of W_G is at least $l+1$, and therefore that $\mu(G)$ has at least $l+1$ distinct zeros.

This same strategy shows that Theorem 78 has the following corollary.

Corollary 79. *Let i and j be vertices in the graph G. Then,*

$$|F_G^i \cap F_G^j| = \dim W_G^i \cap W_G^j \geq \dim W_G^{i,j}.$$

In particular, if there exists a path $c : i \to j$ of length k, then i and j flash simultaneously at least $k+1$ times.

The Corollary 79 gives another proof of the second part of Lemma 65, but does not prove that a path of length $k-1$ has entry equal to one at least k times.

Observe that in the proof of Theorem 76 we have associated with the vector space of polynomials V_G^i a matrix with evaluations of some polynomials using a vandermonde matrix. This type of characterization of vector spaces of polynomials can also be combined with the following lemma.

Lemma 80. *Let M be an n by m matrix, where $n \leq m$, with rank equal to n. If J and K are subsets of $[n]$ and $[m]$, respectively, with $|J| + |K| > m$, then there exists (j,k) in $J \times K$ with $(M)_{j,k}$ different from zero.*

The next result illustrates what may be obtained by combining Theorem 78, the characterization of vector spaces of polynomials alluded to above, and Lemma 80.

Corollary 81. *Let i be a vertex in the graph G that flashes m times. Then there exists a set of paths $\{c_j\}_{j \in [m]}$ in $[i \to \cdot]$ with $\{\mu(G \setminus c_j)\}_{j \in [m]}$ linear independent. In this case, the determinant $\det(\mu(G \setminus c_j)(\theta_k))_{j,k \in [m]}$ is different from zero for every choice of distinct complex numbers $\theta_1, \ldots, \theta_m$ that are not zeros of $\mu(G)$. In particular, if J and K are subsets of $[m]$ with $|J| + |K| > m$, then there exists (j,k) in $J \times K$ with $\mu(G \setminus c_j)(\theta_k)$ different from zero.*

4.3.2 Path Continued Fraction

In this section we present formulas for the path continued fraction of a quotient of characteristic polynomials and graph continued fractions. These formulas allow us to recover some classic results of the theory of distance regular graphs and prove analogous results to matching polynomials. In particular, we prove a new upper bound for the number of paths starting at some vertex i of a graph G using only the matching polynomials of G and $G \setminus i$.

The path continued fraction of a quotient of characteristic polynomials $\dfrac{\phi(G)}{\phi(G \setminus i)}$ can be calculated using the formulas in Section 4.1 and the classic Cauchy-Binet formula.

Proposition 82 (Cauchy-Binet formula)**.** *Let M and N be $m \times n$ and $n \times m$ matrices, respectively. Then,*

$$\det MN = \sum_{\{i_1,\ldots,i_m\}\subseteq[n]} \det \begin{bmatrix} (M)_{1,i_1} & \cdots & (M)_{1,i_m} \\ \vdots & \ddots & \vdots \\ (M)_{m,i_1} & \cdots & (M)_{m,i_m} \end{bmatrix} \cdot \begin{bmatrix} (N)_{i_1,1} & \cdots & (N)_{i_1,m} \\ \vdots & \ddots & \vdots \\ (N)_{i_m,1} & \cdots & (N)_{i_m,m} \end{bmatrix}.$$

The following corollary of Proposition 82 will be the main ingredient in the calculation of the path continued fractions.

Corollary 83. *Let A and B be $n \times n$ matrices, and consider $s_1, \ldots, s_m$ and $t_1, \ldots, t_m$ in $\mathbb{N} \cup \{0\}$ and i in $[n]$. Then,*

$$\det \begin{bmatrix} (A^{s_1}B^{t_1})_{i,i} & \cdots & (A^{s_m}B^{t_1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A^{s_1}B^{t_m})_{i,i} & \cdots & (A^{s_m}B^{t_m})_{i,i} \end{bmatrix} =$$

$$= \sum_{\{i_1,\ldots,i_m\}\subseteq[n]} \det \begin{bmatrix} (A^{s_1})_{i,i_1} & \cdots & (A^{s_1})_{i,i_m} \\ \vdots & \ddots & \vdots \\ (A^{s_m})_{i,i_1} & \cdots & (A^{s_m})_{i,i_m} \end{bmatrix} \cdot \begin{bmatrix} (B^{t_1})_{i_1,i} & \cdots & (B^{t_m})_{i_1,i} \\ \vdots & \ddots & \vdots \\ (B^{t_1})_{i_m,i} & \cdots & (B^{t_m})_{i_m,i} \end{bmatrix}.$$

Proof. Consider the $m \times n$ and $n \times m$ matrices M and N given by $(M)_{j,k} = (A^{s_j})_{i,k}$ and $(N)_{k,j} = (B^{t_j})_{k,i}$, respectively, and apply Proposition 82. $\square$

The determinants in Corollary 83 also have a combinatorial interpretation in terms of non-intersecting walks using the Lindström-Gessel-Viennot-Karlin-McGregor Lemma presented in [49, p.1, Thm. 1], [68, p. 1] and [1, p. 195]. The interpretation in the work of Karlin and McGregor [68] is similar in spirit with what we have in mind. Generalizations of this kind of interpretation also appear under the name of *transfer matrix argument* [22, p. 3-7].

We are now able to compute the path continued fraction of a quotient of characteristic polynomials. In this section, for ease of notation, we write the adjacency matrix of G evaluated at zero, $A_G(0)$, simply as A_G. The next result seems to be new.

Theorem 84 (Path continued fraction for a quotient of characteristic polynomials)**.** *Let i be a vertex in the graph G with vertex set $[n]$. Then,*

$$\frac{\phi(G)}{\phi(G \setminus i)}(x) = x - r_1 + \cfrac{d_1}{x - r_2 + \cfrac{d_2}{\ddots + \cfrac{d_{n-1}}{x - r_n}}},$$

where, for every k in $[n]$,

$$\Delta_k = (-1)^{\frac{(k-1)k}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^{1} = \sum_{\{i_1,\ldots,i_k\}\subseteq[n]} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} \end{bmatrix}^2,$$

and,

$$r_k = \frac{g_k^T A_G g_k}{g_k^T g_k}, \qquad g_k^T g_k = \Delta_k \Delta_{k-1},$$

with,

$$(g_k)_j := \det \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^0)_{i,j} & \cdots & (A_G^{k-1})_{i,j} \end{bmatrix} =$$

$$= \sum_{\{i_1,\dots,i_{k-1}\}\subseteq[n]} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_{k-1}} & \cdots & (A_G^{k-1})_{i,i_{k-1}} \\ (A_G^0)_{i,j} & \cdots & (A_G^{k-1})_{i,j} \end{bmatrix} \cdot \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-2})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_{k-1}} & \cdots & (A_G^{k-2})_{i,i_{k-1}} \end{bmatrix},$$

for every j in $[n]$.

Proof. By Theorem 7 and the formulas of Section 4.1, we can write:

$$\frac{\phi(G\setminus i)}{\phi(G)}(x) = \sum_{m\geq 0} \frac{(-1)^m (A_G^m)_{i,i}}{x^{m+1}} = \cfrac{\tau_0}{x - r_1 + \cfrac{d_1}{x - r_2 + \cfrac{d_2}{\ddots + \cfrac{d_{n-1}}{x - r_n}}}},$$

where,

$$\Delta_k = (-1)^{\frac{(k-1)k}{2}} \tau_0^k d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1 =$$

$$= \det \begin{bmatrix} (A_G^0)_{i,i} & -(A_G^1)_{i,i} & \cdots & (-1)^{k-1}(A_G^{k-1})_{i,i} \\ -(A_G^1)_{i,i} & (A_G^2)_{i,i} & \cdots & (-1)^k (A_G^k)_{i,i} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{k-1}(A_G^{k-1})_{i,i} & (-1)^k (A_G^k)_{i,i} & \cdots & (A_G^{2k-2})_{i,i} \end{bmatrix},$$

and,

$$\chi_k = (r_1 + \cdots + r_k)\Delta_k =$$

$$= \det \begin{bmatrix} (A_G^0)_{i,i} & -(A_G^1)_{i,i} & \cdots & (-1)^{k-1}(A_G^{k-1})_{i,i} \\ -((A_G^1)_{i,i} & (A_G^2)_{i,i} & \cdots & (-1)^k (A_G^k)_{i,i} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^{k-2}(A_G^{k-2})_{i,i} & (-1)^{k-1}(A_G^{k-1})_{i,i} & \cdots & -(A_G^{2k-3})_{i,i} \\ (-1)^k (A_G^k)_{i,i} & (-1)^{k+1}(A_G^{k+1})_{i,i} & \cdots & -(A_G^{2k-1})_{i,i} \end{bmatrix},$$

for every k in $[n]$.

Notice that by multiplying the even rows and columns of the determinant Δ_k and using that $\tau_0 = (-1)^0 (A_G^0)_{i,i} = 1$, we may simplify the formula for Δ_k to obtain,

$$\Delta_k = (-1)^{\frac{(k-1)k}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1 = \det \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-1})_{i,i} & \cdots & (A_G^{2k-2})_{i,i} \end{bmatrix}.$$

Now, applying the Corollary 83 with A and B both equal to $A_G(0)$, s_j and t_j both equal to $j-1$ for every j in $[k]$, and using that $A_G(0)$ is symmetric, it follows that Δ_k is equal to,

$$(-1)^{\frac{(k-1)k}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1 = \sum_{\{i_1,\ldots,i_k\} \subseteq [n]} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} \end{bmatrix}^2.$$

This proves the first equality of the statement. The second and third equalities follow from a more general equality.

First, notice that by multiplying the rows and columns of the determinant χ_k it follows that:

$$\chi_k = \det \begin{bmatrix} (A_G^0)_{i,i} & (A_G^1)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ (A_G^1)_{i,i} & (A_G^2)_{i,i} & \cdots & (A_G^k)_{i,i} \\ \vdots & \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & (A_G^{k-1})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^k)_{i,i} & (A_G^{k+1})_{i,i} & \cdots & (A_G^{2k-1})_{i,i} \end{bmatrix}.$$

Now, let D_k^j be the matrix,

$$D_k^j := \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^0)_{i,j} & \cdots & (A_G^{k-1})_{i,j} \end{bmatrix},$$

so that $(g_k)_j$ equals $\det D_k^j$ by definition. Denote by $D_k^j[k,s]$ the matrix obtained by deleting the row k and column s from D_k^j. Observe that $D_k^j[k,s]$ is independent of j in $[n]$, $D_k^j[k,k]$ equals Δ_{k-1} and $D_k^j[k,k-1]$ equals χ_{k-1}. We proceed as follows:

$$g_k^T A_G^s g_k = \sum_{j,m \in [n]} (g_k)_j (A_G^s)_{j,m} (g_k)_m = \sum_{j,m \in [n]} (A_G^s)_{j,m} \det D_k^j \det D_k^m =$$

$$= \sum_{j,m \in [n]} (A_G^s)_{j,m} \sum_{r,t \in [k]} (-1)^{2k+r+t-4} (A_G^{r-1})_{i,j} \det D_k^j[k,r] (A_G^{t-1})_{i,m} \det D_k^m[k,t] =$$

$$= \sum_{r,t\in[k]} (-1)^{2k+r+t-4} \det D_k^i[k,r] \det D_k^i[k,t] \sum_{j,m\in[n]} (A_G^{r-1})_{i,j}(A_G^s)_{j,m}(A_G^{t-1})_{m,i} =$$

$$= \sum_{r,t\in[k]} (-1)^{2k+r+t-4} \det D_k^i[k,r] \det D_k^i[k,t](A_G^{r+s+t-2})_{i,i} =$$

$$= \sum_{r\in[k]} (-1)^{k+r-2} \det D_k^i[k,r] \sum_{t\in[k]} (-1)^{k+t-2}(A_G^{r+s+t-2})_{i,i} \det D_k^i[k,t] =$$

$$= \sum_{r\in[k]} (-1)^{k+r-2} \det D_k^i[k,r] \det \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^{r+s-1})_{i,i} & \cdots & (A_G^{r+s+k-2})_{i,i} \end{bmatrix} =$$

$$= \sum_{\substack{r\in[k] \\ r\geq k-s}} (-1)^{k+r-2} \det D_k^i[k,r] \det \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^{r+s-1})_{i,i} & \cdots & (A_G^{r+s+k-2})_{i,i} \end{bmatrix}.$$

As a consequence,

$$g_k^T A_G^s g_k = \sum_{\substack{r\in[k] \\ r\geq k-s}} (-1)^{k+r-2} \det D_k^i[k,r] \det \begin{bmatrix} (A_G^0)_{i,i} & \cdots & (A_G^{k-1})_{i,i} \\ \vdots & \ddots & \vdots \\ (A_G^{k-2})_{i,i} & \cdots & (A_G^{2k-3})_{i,i} \\ (A_G^{r+s-1})_{i,i} & \cdots & (A_G^{r+s+k-2})_{i,i} \end{bmatrix},$$

for every s in $\mathbb{N}\cup\{0\}$. Plugging s equal to 0 in this last equality, it immediately follows that $g_k^T g_k$ equals $\Delta_k\Delta_{k-1}$, which proves the third equality of the statement. Applying the above with s equal to 1 and using the formulas of Section 4.1, it follows that,

$$r_k = \frac{\chi_k\Delta_{k-1} - \chi_{k-1}\Delta_k}{\Delta_k\Delta_{k-1}} = \frac{g_k^T A_G g_k}{g_k^T g_k},$$

proving the second equality of the statement.

Finally, observe that the last equality of the statement, with the definition of $(g_k)_j$, is a consequence of Proposition 82. □

Observe that the Theorem 84 also shows that the coefficients r_k and d_k in the path continued fraction of $\dfrac{\phi(G)}{\phi(G \setminus i)}$ only depend on the k-neighborhood of i, i.e., the vertices which are at distance less than, or equal to, k from i.

Using a modification of Corollary 83 and the same proof strategy of Theorem 84 one can give a formula for the path continued fraction,

$$\sum_{i\in I}\frac{\phi(G\setminus i)}{\phi(G)}(x)=\cfrac{|I|}{x-r_1+\cfrac{d_1}{x-r_2+\cfrac{d_2}{\ddots+\cfrac{d_{n-1}}{x-r_n}}}},$$

where I is a subset of $[n]$.

As a particular case of such result there is the following formula for the path continued fraction of the logarithmic derivative of a characteristic polynomial.

Theorem 85 (Path continued fraction of the logarithmic derivative of a characteristic polynomial)**.** *Let G be a graph with vertex set $[n]$. Then,*

$$\frac{\phi(G)'}{\phi(G)}(x)=\cfrac{n}{x-r_1+\cfrac{d_1}{x-r_2+\cfrac{d_2}{\ddots+\cfrac{d_{n-1}}{x-r_n}}}},$$

where, for every k in $[n]$,

$$\Delta_k=(-1)^{\frac{(k-1)k}{2}}n^k d_1^{k-1}d_2^{k-2}\cdots d_{k-1}^{1}=$$

$$=\sum_{\{(i_1,j_1),\dots,(i_k,j_k)\}\subseteq[n]\times[n]}\det\begin{bmatrix}(A_G^0)_{i_1,j_1} & \cdots & (A_G^{k-1})_{i_1,j_1}\\ \vdots & \ddots & \vdots\\ (A_G^0)_{i_k,j_k} & \cdots & (A_G^{k-1})_{i_k,j_k}\end{bmatrix}^2,$$

and,

$$r_k=\frac{g_k^TA_Gg_k}{g_k^Tg_k},\qquad g_k^Tg_k=\Delta_k\Delta_{k-1},$$

with,

$$(g_k)_j:=\det\begin{bmatrix}\sum_{i\in[n]}(A_G^0)_{i,i} & \cdots & \sum_{i\in[n]}(A_G^{k-1})_{i,i}\\ \vdots & \ddots & \vdots\\ \sum_{i\in[n]}(A_G^{k-2})_{i,i} & \cdots & \sum_{i\in[n]}(A_G^{2k-3})_{i,i}\\ \sum_{i\in[n]}(A_G^0)_{i,j} & \cdots & \sum_{i\in[n]}(A_G^{k-1})_{i,j}\end{bmatrix},$$

for every j in $[n]$.

The k-subdiscriminant of a monic polynomial p of degree n, with $n > k \geq 0$, in $\mathbb{C}[x]$ is defined as follows. Let $x_1, \ldots, x_n$ be the multiset of zeros of p in $\mathbb{C}[x]$. Then the k-subdiscriminant of p is by definition,

$$SubDisc_k(p) := \sum_{\substack{I \subseteq [n] \\ |I| = n-k}} \prod_{\{i,j\} \subseteq I} (x_i - x_j)^2.$$

Subdiscriminants generalize the classic notion of discriminant. Observe that the 0-subdiscriminant is the usual discriminant, and that $SubDisc_k(p)$ is different from zero if, and only if, p has at least $n - k$ distinct zeros.

Using the formulas of Section 4.1 it is not difficult to see that the expression Δ_k in the Theorem 85 is equal to the $(n-k)$-subdiscriminant of the characteristic polynomial $\phi(G)$, i.e.,

$$SubDisc_{n-k}(\phi(G)) = \Delta_k.$$

But this last expression in Theorem 85 is actually a sum of squares. Using a combinatorial interpretation for Corollary 83 in terms of non-intersecting walks then leads to a combinatorial proof of a result in [95, p. 3, Prop. 4], that all the subdiscriminants of the characteristic polynomial of a matrix can be written as a sum of squares.

It is also interesting to note that the best result up to date in Domokos' work [33, p. 453, Thm. 6.2] writes the discriminant Δ_n of an $n \times n$ symmetric matrix as the sum of $\binom{2n-1}{n-1} - \binom{2n-3}{n-1}$ squares. On the other hand, as seen in Theorem 85, the product $\Delta_n \Delta_{n-1}$ (which is different from zero if, and only if, $\Delta_n \neq 0$) can be written as the sum of just n squares.

The same reasoning presented above proves that for every graph G and subset I of $[n]$, the resultant of $\phi(G)$ and $\sum_{i \in I} \phi(G \setminus i)$ is also a sums of squares.

In the next result we show how the formula of Theorem 84 is related to the diameter of a graph. Given a vertex i in the graph G and a natural number k, denote by S^i_k the set of vertices of G that are at distance k from i. It is useful to denote by S^i_0 the set $\{i\}$.

Theorem 86 (Quotient of characteristic polynomials and diameter)**.** *Let i be a vertex in the graph G, and consider the path continued fraction for $\dfrac{\phi(G)}{\phi(G \setminus i)}$. Then,*

$$(-1)^k d_1 d_2 \cdots d_k \geq \sum_{j \in S^i_k} (A^k_G)^2_{i,j} \geq \frac{1}{|S^i_k|} \left(\sum_{j \in S^i_k} (A^k_G)_{i,j} \right)^2,$$

for every k in $[n]$.

Proof. Let j be in S^i_k. First notice that $(A^m_G(0))_{i,j}$ is equal to 0 if m is smaller than k. This implies that for every subset $\{i_1, \ldots, i_k\}$ of $[n]$ it holds,

$$\det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} & (A_G^k)_{i,i_1} \\ \vdots & \ddots & \vdots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} & (A_G^k)_{i,i_k} \\ (A_G^0)_{i,j} & \cdots & (A_G^{k-1})_{i,j} & (A_G^k)_{i,j} \end{bmatrix}^2 =$$

$$= (A_G^k)_{i,j}^2 \cdot \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} \end{bmatrix}^2 .$$

Also notice that if $\{i_1, \ldots, i_k\}$ contains an element of S_k^i then this last determinant is 0. Putting this all together it follows by Theorem 84 that,

$$(-1)^k d_1 d_2 \cdots d_k = \frac{(-1)^{\frac{(k-1)k}{2}} d_1^k d_2^{k-1} \cdots d_{k-1}^2 d_k^1}{(-1)^{\frac{(k-2)(k-1)}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1} \geq$$

$$\geq \frac{\displaystyle\sum_{\substack{\{i_1,\ldots,i_{k+1}\}\subseteq[n] \\ i_{k+1}\in S_k^i}} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^k)_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_{k+1}} & \cdots & (A_G^k)_{i,i_{k+1}} \end{bmatrix}^2}{(-1)^{\frac{(k-2)(k-1)}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1} =$$

$$= \frac{\displaystyle\sum_{j\in S_k^i} \sum_{\{i_1,\ldots,i_k\}\subseteq[n]} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} & (A_G^k)_{i,i_1} \\ \vdots & \ddots & \vdots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} & (A_G^k)_{i,i_k} \\ (A_G^0)_{i,j} & \cdots & (A_G^{k-1})_{i,j} & (A_G^k)_{i,j} \end{bmatrix}^2}{(-1)^{\frac{(k-2)(k-1)}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1} =$$

$$= \frac{\displaystyle\sum_{j\in S_k^i} (A_G^k)_{i,j}^2 \sum_{\{i_1,\ldots,i_k\}\subseteq[n]} \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A_G^0)_{i,i_k} & \cdots & (A_G^{k-1})_{i,i_k} \end{bmatrix}^2}{(-1)^{\frac{(k-2)(k-1)}{2}} d_1^{k-1} d_2^{k-2} \cdots d_{k-1}^1} =$$

$$= \sum_{j\in S_k^i} (A_G^k)_{i,j}^2 \geq \frac{1}{|S_k^i|} \left(\sum_{j\in S_k^i} (A_G^k)_{i,j} \right)^2 ,$$

where this last inequality is Cauchy-Schwarz. □

It follows from Theorem 86 the well known fact that $\phi(G)$ has at least $diam(G)+1$ zeros, and that $\dfrac{\phi(G)}{\phi(G \setminus i)}$ has at least $\dfrac{diam(G)}{2} + 1$ zeros for every vertex i of the graph G.

The really interesting part about the inequality in Theorem 86 are the conditions that guarantee equality up to some point, as the next results show.

Theorem 87. *Let i be a vertex in the graph G with S^i_{m-1} non-empty, and consider the path continued fraction for $\dfrac{\phi(G)}{\phi(G \setminus i)}$. Then the following are equivalent:*

a) $(-1)^k d_1 d_2 \cdots d_k = \sum_{j \in S^i_k} (A^k_G)^2_{i,j}$, *for every k in $[m]$;*

b) The vectors $((A^k_G)_{i,j_1})_{k\in[m]}$ and $((A^k_G)_{i,j_2})_{k\in[m]}$ are scalar multiples for every j_1 and j_2 which are in a same component of the partition $S^i_1 \sqcup \cdots \sqcup S^i_{m-1}$.

Proof. Observe that implicit in the proof of Theorem 86, the equality,

$$(-1)^k d_1 d_2 \cdots d_k = \sum_{j \in S^i_k} (A^k_G)^2_{i,j},$$

holds for some k if, and only if,

$$\sum_{\{i_1,\ldots,i_{k+1}\}\subseteq S^i_0 \sqcup S^i_1 \sqcup \cdots \sqcup S^i_{k-1}} \det \begin{bmatrix} (A^0_G)_{i,i_1} & \cdots & (A^k_G)_{i,i_1} \\ \vdots & \ddots & \vdots \\ (A^0_G)_{i,i_{k+1}} & \cdots & (A^k_G)_{i,i_{k+1}} \end{bmatrix}^2 = 0.$$

First, we prove that (b) implies (a). Consider k in $[m]$ and observe that by the Pigeonhole Principle, for every choice of subset $\{i_1, \ldots, i_{k+1}\}$ of $S^i_0 \sqcup S^i_1 \sqcup \cdots \sqcup S^i_{k-1}$ there are two distinct elements i_r and i_s which are in a same component of the partition. By the assumption of item (b), $((A^k_G)_{i,i_r})_{k\in[m]}$ and $((A^k_G)_{i,i_s})_{k\in[m]}$ are scalar multiples. This implies that the determinant of $((A^{t-1}_G)_{i,i_j})_{(t,j)\in[k]\times[k]}$ is zero. Since the subset $\{i_1, \ldots, i_{k+1}\}$ is arbitrary, it follows that,

$$\sum_{\{i_1,\ldots,i_{k+1}\}\subseteq S^i_0 \sqcup S^i_1 \sqcup \cdots \sqcup S^i_{k-1}} \det((A^{t-1}_G)_{i,i_j})^2_{(t,j)\in[k]\times[k]} = 0,$$

which, by the criteria above, shows that there is equality in the item (a) for the given k.

We now prove that (a) implies (b). Let j_1 and j_2 be two vertices in a same component S^i_t of the partition $S^i_1 \sqcup \cdots \sqcup S^i_{m-1}$. In this case, both $(A^k_G)_{i,j_1}$ and $(A^k_G)_{i,j_2}$ are zero for k smaller than t, and both $(A^t_G)_{i,j_1}$ and $(A^t_G)_{i,j_2}$ are non-zero. We will prove by induction in k that $(A^k_G)_{i,j_2}$ equals $\dfrac{(A^t_G)_{i,j_2}}{(A^t_G)_{i,j_1}}(A^k_G)_{i,j_1}$ for every k in $\{0, \cdots, m\}$. This is clearly true for k smaller than, or equal to, t, so assume k is in $\{t+1, \cdots, m\}$.

Since S^i_{k-1} is non-empty we can consider $i_1, \ldots, i_k$ in $S^i_0, \ldots, S^i_{k-1}$, respectively, with i_{t+1} equal to j_1. Then, by the criteria above for the equality in item (a) for k and the induction hypothesis,

$$0 = \det \begin{bmatrix} (A^0_G)_{i,i_1} & \cdots & (A^{k-1}_G)_{i,i_1} & (A^k_G)_{i,i_1} \\ \vdots & \ddots & \vdots & \vdots \\ (A^0_G)_{i,i_k} & \cdots & (A^{k-1}_G)_{i,i_k} & (A^k_G)_{i,i_k} \\ (A^0_G)_{i,j_2} & \cdots & (A^{k-1}_G)_{i,j_2} & (A^k_G)_{i,j_2} \end{bmatrix}^2 =$$

$$= \det \begin{bmatrix} (A_G^0)_{i,i_1} & \cdots & (A_G^{k-1})_{i,i_1} & (A_G^k)_{i,i_1} \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \ddots & (A_G^{k-1})_{i,i_k} & (A_G^k)_{i,i_k} \\ 0 & \cdots & 0 & (A_G^k)_{i,j_2} - \dfrac{(A_G^t)_{i,j_2}}{(A_G^t)_{i,j_1}}(A_G^k)_{ij_1} \end{bmatrix}^2 =$$

$$= (A_G^0)_{i,i_1}^2 \cdots (A_G^{k-1})_{i,i_k}^2 \left((A_G^k)_{i,j_2} - \frac{(A_G^t)_{i,j_2}}{(A_G^t)_{i,j_1}}(A_G^k)_{ij_1} \right)^2 \implies$$

$$(A_G^k)_{i,j_2} = \frac{(A_G^t)_{i,j_2}}{(A_G^t)_{i,j_1}}(A_G^k)_{ij_1}.$$

This proves the induction step and finishes the proof. □

We say that S_r^i *sends same weight* to S_t^i if the sum $\sum_{j \in S_t^i} (A_G)_{v,j}$ is constant as v varies in S_r^i, and if this constant is equal to w then we say S_r^i sends weight w to S_t^i. Observe that this definition is meaningful only if $|r - t|$ is at most one.

Theorem 88. *Let i be a vertex in the graph G with S_{m-1}^i non-empty, and consider the path continued fraction for $\dfrac{\phi(G)}{\phi(G \setminus i)}$. Then the following are equivalent:*

a) $(-1)^k d_1 d_2 \cdots d_k = \dfrac{1}{|S_k^i|} \left(\sum_{j \in S_k^i} (A_G^k)_{i,j} \right)^2$*, for every k in $[m]$;*

b) $((A_G^k)_{i,j})_{k \in [m]}$ *only depends on the component of j in the partition $S_1^i \sqcup \cdots \sqcup S_m^i$;*

c) *S_k sends same weight to S_{k-1}, S_k and S_{k+1} for every k in $0 \sqcup [m-2]$, S_{m-1} sends same weight to S_{m-2} and S_{m-1}, and S_m sends same weight to S_{m-1}.*

Furthermore, if one of these conditions is satisfied, then,

$$(-1)^k d_1 d_2 \cdots d_k = |S_k^i| (A_G^k)_{i,j}^2,$$

for every k in $[m]$ and j in S_k^i. Also, S_{k-1}^i sends weight r_k to S_{k-1}^i for every k in $[m]$, and $-d_k$ is the product of the weights that S_{k-1}^i sends to S_k^i and S_k^i sends to S_{k-1}^i, for every k in $[m-1]$.

Proof. We prove that (a) is equivalent to (b), and (b) is equivalent to (c). Assume that (a) holds, then, since there is equality in the Cauchy-Schwarz inequality of Theorem 86, it follows that $(A_G^t)_{i,j_1}$ is equal to $(A_G^t)_{i,j_2}$ for every j_1 and j_2 which are in a same component S_t^i with t in $[m]$. But, by the equivalence in Theorem 87, $((A_G^k)_{i,j_1})_{k \in [m]}$ and $((A_G^k)_{i,j_2})_{k \in [m]}$ are scalar multiples for every j_1 and j_2 which are in a same component of the partition $S_1^i \sqcup \cdots \sqcup S_{m-1}^i$. It follows that $((A_G^k)_{i,j_1})_{k \in [m]}$ and $((A_G^k)_{i,j_2})_{k \in [m]}$ are in fact equal for every j_1 and j_2 which are in a same component of the partition $S_1^i \sqcup \cdots \sqcup S_m^i$. This proves that (a) implies (b).

Now suppose that (b) is valid. Then, by the equivalence in Theorem 87 it follows that, for every k in $[m]$,

$$(-1)^k d_1 d_2 \cdots d_k = \sum_{j \in S_k^i} ((A_G^k)_{i,j})^2 = \frac{1}{|S_k^i|} \left(\sum_{j \in S_k^i} (A_G^k)_{i,j} \right)^2 ,$$

where the second equality is because $(A_G^k)_{i,j_1}$ is equal to $(A_G^k)_{i,j_2}$ for every j_1 and j_2 in S_k^i. This proves that (b) implies (a).

The proof that (b) is equivalent to (c) follows from the equality:

$$(A_G^t)_{i,v} = \sum_{j \in S_{k-1}^i} (A_G^{t-1})_{i,j} (A_G)_{j,v} + \sum_{j \in S_k^i} (A_G^{t-1})_{i,j} (A_G)_{j,v} + \sum_{j \in S_{k+1}^i} (A_G^{t-1})_{i,j} (A_G)_{j,v},$$

for every t in $[m]$ and k in $\{0\} \sqcup [m]$, where v is in S_k^i.

Assume that (b) holds. Then, for any given k in $[m]$, using the equality above for t equal to k and v in S_k^i, one can prove that S_k sends same weight to S_{k-1}. Using this information and the equality above for t equal to $k+1$ and smaller than m, and v in S_k^i, it follows that S_k^i sends same weight to S_k^i for every k in $\{0\} \cup [m-1]$. Finally, by these observations and the equality above for t equal to $k+2$ and smaller than m, and v in S_k^i, it follows that S_k^i sends same weight to S_{k+1}^i for every k in $\{0\} \cup [m-2]$. This shows that (b) implies (c).

Now suppose that (c) is valid. We will prove by induction in t that for t in $\{0\} \cup [m]$, $(A_G^t)_{i,v}$ only depends on the component of v in $S_0^i \sqcup \cdots \sqcup S_k^i$. Observe that this is clearly true for t equal to zero. The induction step is true because by the equation above, $(A^t)_{i,v}$ for t in $\{0\} \cup [m]$ only depends in the entries of the matrices $A, \ldots, A^{t-1}$ and the weights that the components of $S_0^i, \cdots, S_k^i$ send to each other as described in item (c). This shows that (c) implies (b).

For the last part of the statement, observe that the items (a) and (b) together imply,

$$(-1)^k d_1 d_2 \cdots d_k = |S_k^i| (A_G^k)_{i,j}^2,$$

for every k in $[m]$ and j in S_k^i. Now consider j_1 in S_{k-1}^i and v_1 in S_k^i. Note that if S_k and S_{k-1} both send same weight to each other, then,

$$|S_{k-1}^i| \sum_{v \in S_k^i} (A_G)_{j_1,v} = \sum_{j \in S_{k-1}^i, v \in S_k^i} (A_G)_{j,v} = |S_k^i| \sum_{j \in S_{k-1}^i} (A_G)_{v_1,j}.$$

As a consequence,

$$-d_k = \frac{|S_k^i| (A_G^k)_{i,v_1}^2}{|S_{k-1}^i| (A_G^{k-1})_{i,j_1}^2} = \frac{|S_k^i| \left(\sum_{j \in S_{k-1}^i} (A_G^{k-1})_{i,j} (A_G)_{j,v_1} \right)^2}{|S_{k-1}^i| (A_G^{k-1})_{i,j_1}^2} =$$

$$= |S^i_{k-1}||S^i_k| \left(\sum_{j \in S^i_{k-1}} (A_G)_{j,v_1} \right)^2 = \left(\sum_{v \in S^i_{k-1}} (A_G)_{j_1,v} \right) \left(\sum_{j \in S^i_k} (A_G)_{v_1,j} \right).$$

This proves that $-d_k$ is the product of the weights that S^i_{k-1} sends to S^i_k and S^i_k sends to S^i_{k-1}, for every k in $[m-1]$.

From the item (b) and the Theorem 84 it follows that, for every k in $[m+1]$, $(g_k)_j$ equals $(A^{k-1}_G)_{i,j}\Delta_{k-1}$ for every j in S^i_{k-1} and zero otherwise. As a consequence, for every k in $[m]$,

$$r_k = \frac{g^T_k A_G g_k}{g^T_k g_k} = \frac{\sum_{j,v \in S^i_{k-1}} (A_G)_{j,v} (A^{k-1}_G)_{i,j} (A^{k-1}_G)_{i,v} \Delta^2_{k-1}}{\Delta_k \Delta_{k-1}} = \frac{\sum_{j \in S^i_{k-1}} (A^{k-1}_G)^2_{i,j} \sum_{v \in S^i_{k-1}} (A_G)_{j,v}}{(-1)^{k-1} d_1 d_2 \cdots d_{k-1}} =$$

$$= \sum_{v \in S^i_{k-1}} (A_G)_{j_1,v},$$

where j_1 is in S^i_{k-1}. This proves that r_k is equal to the weight that S^i_{k-1} sends to S^i_{k-1} for every k in $[m]$. □

For *distance-regular graphs* there is always equality in the Theorem 88. In fact, the equivalent items of this theorem are inspired by the properties of distance-regular graphs. The Theorem 88 is a simplified weighted version of results which originally appear in the work of Fiol, Garriga and Yebra [39–41], providing a local characterization of distance-regularity. For a nice overview of the theory of distance-regular graphs one can read Godsil's book [52, p. 195-217, Chpt. 11].

In the case of d-regular graphs one can do slightly better in Theorem 88 and compute the number of vertices in each sphere S^i_k.

Corollary 89. *Consider a d-regular graph G with vertex weights x and edge weights -1. Let i be a vertex in G with S^i_{m-1} non-empty and assume that the path continued fraction of $\frac{\phi(G)}{\phi(G \setminus i)}$ satisfies one of the equivalent statements of Theorem 88. Then $|S^i_k|$ can be computed from the path continued fraction for every k in $[m]$.*

Proof. First notice that, since G is d-regular, one can prove using Theorem 88 and the last part of its proof that S^i_{m-1} sends same weight to S^i_m and $-d_m$ is the product of the weights that S^i_{m-1} sends to S^i_m and S^i_m sends to S^i_{m-1}. Denote by p_{k+1} the weight that S^i_k sends to S^i_{k-1} for every k in $[m]$, and by s_{k+1} the weight that S_k sends to S^i_{k+1} for every k in $\{0\} \cup [m-1]$. Then one has the relations: $s_1 = d$, $p_{k+1} + r_{k+1} + s_{k+1} = d$ for every k in $[m-1]$, $s_k p_{k+1} = -d_k$ and $|S^i_{k-1}|s_k = p_{k+1}|S^i_k|$ for every k in $[m]$. Using these equations one can compute recursively the values of $|S^i_k|$ for every k in $[m]$. □

Using the proof strategies of Theorems 88 and 89, but with the path continued fraction of the logarithmic derivative of a characteristic polynomial, one can give a proof of a result nowadays known as the *spectral excess theorem* [40, p. 180, Thm. 4.4]. For a simple proof of this theorem and some of its applications we recommend the articles [28, p. 7, Thm. 1] and [42, p. 395, Thm. 2.1].

Now we focus on graph continued fractions. Using the Theorem 84 and Godsil's Lemma 16 we can obtain the path continued fraction of graph continued fractions. This is our main result of this section which is definitely new. Recall from Lemma 27 that for every path c in the graph G we may write,

$$\sum_{m\geq 0} \frac{(-1)^m t_c^m}{x^{m+1}} = \sqrt{\lambda_c}\frac{\mu(G\setminus c)}{\mu(G)}(x),$$

where t_c^m is the number of walks from the root i to the vertex corresponding to the path c in the path tree T_G^i.

Theorem 90 (Path continued fraction of a graph continued fraction)**.** *Let i be a vertex in the graph G with vertex set $[n]$. Then,*

$$\alpha_i(G)(x) = x - r_1 + \cfrac{d_1}{x - r_2 + \cfrac{d_2}{\ddots + \cfrac{d_{n-1}}{x - r_n}}},$$

where, for every k in $[n]$,

$$\Delta_k = (-1)^{\frac{(k-1)k}{2}} d_1^{k-1} d_2^{k-2}\cdots d_{k-1}^1 = \sum_{\{c_1,\dots,c_k\}\subseteq[i\to\cdot]} \det\begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-1} \\ \vdots & \ddots & \vdots \\ t_{c_k}^0 & \cdots & t_{c_k}^{k-1}\end{bmatrix}^2,$$

and,

$$r_k = \frac{g_k^T A_{T_G^i} g_k}{g_k^T g_k}, \qquad g_k^T g_k = \Delta_k \Delta_{k-1},$$

with,

$$(g_k)_c := \det\begin{bmatrix} t_i^0 & \cdots & t_i^{k-1} \\ \vdots & \ddots & \vdots \\ t_i^{k-2} & \cdots & t_i^{2k-3} \\ t_c^0 & \cdots & t_c^{k-1}\end{bmatrix} =$$

$$= \sum_{\{c_1,\dots,c_{k-1}\}\subseteq[i\to\cdot]} \det\begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-1} \\ \vdots & \ddots & \vdots \\ t_{c_{k-1}}^0 & \cdots & t_{c_{k-1}}^{k-1} \\ t_c^0 & \cdots & t_c^{k-1}\end{bmatrix} \cdot \det\begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-2} \\ \vdots & \ddots & \vdots \\ t_{c_{k-1}}^0 & \cdots & t_{c_{k-1}}^{k-2}\end{bmatrix},$$

for every c in $[i \to \cdot]$.

Proof. Observe that by Lemmas 16 and 24 we may write,

$$\sum_{m\geq 0}\frac{(-1)^m t_i^m}{x^{m+1}} = \alpha_i(G)(x) = \frac{\phi(T_G^i)}{\phi(T_G^i\setminus i)}(x) = \sum_{m\geq 0}\frac{(-1)^m (A_{T_G^i}^m)_{i,i}}{x^{m+1}}.$$

Also notice that by Lemma 27 we have,

$$\sum_{m\geq 0}\frac{(-1)^m t_c^m}{x^{m+1}} = \sqrt{\lambda_c}\frac{\mu(G\setminus c)}{\mu(G)}(x) = \rho_c\frac{\phi(T_G^i\setminus c)}{\phi(T_G^i)}(x) = \sum_{m\geq 0}\frac{(-1)^m (A_{T_G^i}^m)_{i,c}}{x^{m+1}}.$$

The proof then follows from Theorem 84. □

Analogous to the Theorem 85 there is a formula for the logarithmic derivative of matching polynomials. Let $\hat{G}$ be the weighted graph obtained from G by joining a new vertex v with weight x to all the vertices of G trough edges of weight -1. Then, by Lemma 25,

$$\alpha_v(\hat{G})(x) = x - \frac{\mu(G)'}{\mu(G)}(x).$$

Also notice that the set of paths starting at v in $\hat{G}$ is in direct correspondence with the set of all paths in G, and the weights of the paths also correspond under this map. Applying Theorem 90 to $\hat{G}$ we obtain the following corollary.

Corollary 91 (Path continued fraction of the logarithmic derivative of a matching polynomial)**.** *Let G be a graph with vertex set $[n]$. Then,*

$$\frac{\mu(G)'}{\mu(G)}(x) = \cfrac{n}{x - r_1 + \cfrac{d_1}{x - r_2 + \cfrac{d_2}{\ddots + \cfrac{d_{n-1}}{x - r_n}}}},$$

where, for every k in $[n]$,

$$\Delta_k = (-1)^{\frac{(k-1)k}{2}} n^k d_1^{k-1} d_2^{k-2}\cdots d_{k-1}^1 = \sum_{\{c_1,\dots,c_k\}\subseteq[\cdot\to\cdot]} \det\begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-1}\\ \vdots & \ddots & \vdots\\ t_{c_k}^0 & \cdots & t_{c_k}^{k-1}\end{bmatrix}^2,$$

and,

$$r_k = \frac{g_k^T A_{T_{\hat{G}}^v} g_k}{g_k^T g_k}, \qquad g_k^T g_k = \Delta_k\Delta_{k-1},$$

with,

$$(g_k)_c := \det \begin{bmatrix} t_v^0 & \cdots & t_v^{k-1} \\ \vdots & \ddots & \vdots \\ t_v^{k-2} & \cdots & t_v^{2k-3} \\ t_c^0 & \cdots & t_c^{k-1} \end{bmatrix} =$$

$$= \sum_{\{c_1,\ldots,c_{k-1}\}\subseteq[\cdot\to\cdot]} \det \begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-1} \\ \vdots & \ddots & \vdots \\ t_{c_{k-1}}^0 & \cdots & t_{c_{k-1}}^{k-1} \\ t_c^0 & \cdots & t_c^{k-1} \end{bmatrix} \cdot \det \begin{bmatrix} t_{c_1}^0 & \cdots & t_{c_1}^{k-2} \\ \vdots & \ddots & \vdots \\ t_{c_{k-1}}^0 & \cdots & t_{c_{k-1}}^{k-2} \end{bmatrix},$$

for every c in $[\cdot \to \cdot]$.

As a consequence of Corollary 91, the subdiscriminants of matching polynomials can also be written as a sum of squares. This observation about matching polynomials seems to be new. The Theorem 90 and Corollary 91 also provide another perspective on the results of Section 4.3.1.

The Corollary 45 proves that the discriminant of the matching polynomial of a vertex-transitive graph is nonzero. It seems reasonable to conjecture that the discriminant is large for this class of graphs. The zero position of the matching polynomial of vertex-transitive bipartite graphs was also studied in the work of Csikvári [26].

Analogous to Theorem 86, the Theorem 90 implies an upper bound in terms of the matching polynomials of G and $G \setminus i$ for the number of paths with length k starting at the vertex i. The next result seems to be new.

Theorem 92 (Graph continued fraction and paths). *Let i be a vertex in the graph G, and consider the path continued fraction for $\alpha_i(G)$. Then,*

$$(-1)^k d_1 d_2 \cdots d_k \geq \sum_{\substack{c\in[i\to\cdot] \\ l(c)=k}} (A_{T_G^i}^k)_{i,c}^2,$$

for every k in $[n]$. In particular, if all the vertex weights of G are x, then,

$$(-1)^k d_1 d_2 \cdots d_k \geq \sum_{\substack{c\in[i\to\cdot] \\ l(c)=k}} \lambda_c,$$

for every k in $[n]$.

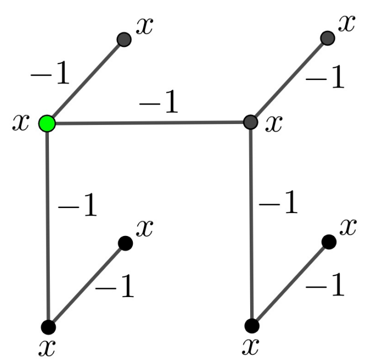
Proof. This is an immediate consequence of Theorem 86 and Godsil's Lemma 16. It is also possible to give a simple proof by induction using only the formulas of Section 4.1. □

The Theorem 92 can be seen as more precise version of Lemma 65 presenting a quantitative connection between paths and matchings. The next two examples present the bounds of Theorem 92 for two graphs.

In general the bound of Theorem 92 is bad, as the next example shows.

Example 93. *Consider the family of graphs of Example 70. Let G be the rooted graph with vertex set $[2]$ where there is and edge between the two vertices and the root is 1. Assume that the vertices weights is x and the edge weights is -1, so that the graph continued fraction of G is $x - \dfrac{1}{x}$. Consider now the sequence of rooted graphs $(G_n)_{n\geq 1}$, where $G_1 = G$ and $G_{n+1} = G_n \circ G$ for n bigger than, or equal to, one. Observe that the root of G_n is a maximum flasher while length of the largest path starting at it is exactly n.*

In Figure 4.2 we present the graph continued fraction for G_3 written as a quotient and path continued fraction.



$$= \frac{x^8 - 7x^6 + 13x^4 - 7x^2 + 1}{x^7 - 4x^5 + 4x^3 - x} =$$

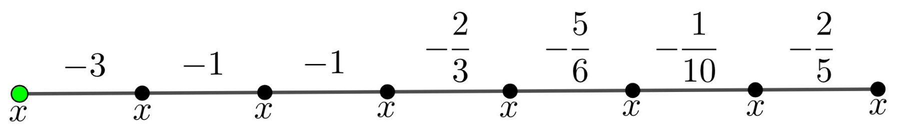
$=$ 

Figure 4.2: Graph continued fraction of the graph G_3 written as a quotient and path continued fraction.

Table 4.1 presents the bounds given by Theorem 92 for G_3.

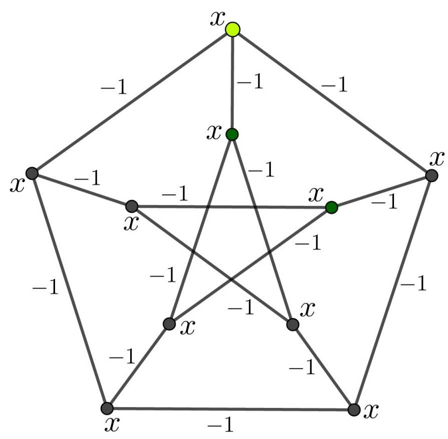
Table 4.1: Bounds of Theorem 92 for the graph G_3.

k	1	2	3	4	5	6	7
$(-1)^k d_1 d_2 \cdots d_k$	3	3	3	2	$\frac{5}{3}$	$\frac{1}{6}$	$\frac{1}{15}$
Paths of length k	3	3	1	0	0	0	0

As n grows the bound of Theorem 92 for G_n becomes worse.

However, for some graphs the bound of Theorem 92 is sharp, as the next example shows.

Example 94 (Petersen graph)**.** *The Petersen graph is a small vertex-transitive graph. In Figure 4.3 we present the graph continued fraction for the Petersen graph written as a quotient and path continued fraction.*



$$= \frac{x^{10} - 15x^8 + 75x^6 - 145x^4 + 90x^2 - 6}{x^9 - 12x^7 + 45x^5 - 58x^3 + 18x} =$$

$=$

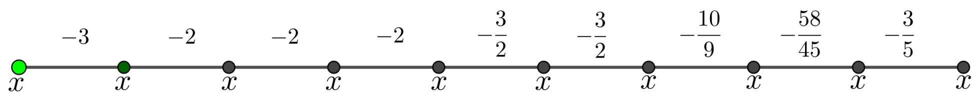


Figure 4.3: Graph continued fraction of the Petersen graph written as a quotient and path continued fraction.

Table 4.2 verifies that the bound of Theorem 92 works for the Petersen graph and is sharp for some path lengths.

Table 4.2: Bounds of Theorem 92 for the Petersen graph.

k	1	2	3	4	5	6	7	8	9
$(-1)^k d_1 d_2 \cdots d_k$	3	6	12	24	36	54	60	$\frac{232}{3}$	$\frac{232}{5}$
Paths of length k	3	6	12	24	36	48	60	60	24

The fact that the bound of Theorem 92 works well for the Petersen graph is not accidental. This happens because there is the analogous statement for graph continued fractions of Theorem 87.

A *non-backtracking walk* in a graph is a walk such that a step is never followed by its inverse, i.e., if the walk is $i_1, i_2, \ldots, i_k$ then i_j is different from i_{j+2} for every j in $[k-2]$. A walk that is not a path, i.e., repeats vertices, is said to *self-intersect*. The next theorem is definitely new.

Theorem 95. *Consider a regular graph G with vertex weights x and edge weights -1. Let i be a vertex in G and consider the path continued fraction for $\alpha_i(G)$. Then, $-d_1$ is equal to the degree of every vertex in G, and, if m is the largest index such that $-d_2, \ldots, -d_{m-1}$ are all equal to $-(d_1 - 1)$, then,*

$$(-1)^k d_1 d_2 \cdots d_k = |\{c \in [i \to \cdot] \mid l(c) = k\}|,$$

for every k in $[m]$. In particular, the total number of shortest non-backtracking walks starting at i that self-intersect is $d(d-1)^m - (-1)^m d_1 d_2 \cdots d_m$.

Proof. Assume that G is a d-regular graph. Let m be the smallest natural number such that there exists a non-backtracking walk starting at i that self intersects. We show that this m satisfies the properties of the statement.

Since $\alpha_i(G)$ equals $\dfrac{\phi(T_G^i)}{\phi(T_G^i \setminus i)}$ their path continued fractions are equal. For this reason, we focus on the path continued fraction of $\dfrac{\phi(T_G^i)}{\phi(T_G^i \setminus i)}$.

Consider the path tree T_G^i, and let S_k^i be the set of vertices of T_G^i that are at distance k from the root i for every k in $\{0\} \cup [m]$. Using the definition of m and the facts that G is d-regular and T_G^i is a tree it follows that: S_0^i sends weight d to S_1^i, S_k^i sends weight $d-1$ to S_{k+1}^i for every k in $[m-2]$, S_k^i sends weight 0 to S_k^i for every k in $\{0\} \cup [m-1]$ and S_k^i sends weight 1 to S_{k-1}^i for every k in $[m]$.

Since T_G^i is a tree with vertex weights x and edge weights -1 there is only a path of weight 1 between every vertex and the root. It then follows by Theorem 88 that,

$$(-1)^k d_1 d_2 \cdots d_k = \frac{1}{|S_k^i|} \left(\sum_{j \in S_k^i} (A^k_{T_G^i})_{i,j} \right)^2 = |S_k^i| = |\{c \in [i \to \cdot] \mid l(c) = k\}|,$$

for every k in $[m]$. By Theorem 88 and the discussion above it holds that $-d_1$ is equal to d and $-d_k$ is equal to $d-1$ for every k in $[m-1]$. Since G is d-regular the total number of non-backtracking walks of length m is $d(d-1)^m$, and by the equality above exactly $(-1)^m d_1 d_2 \cdots d_m$ of these don't self-intersect. By the definition of m there exists a non-backtracking walk of length m that self-intersects, so $d(d-1)^m$ is bigger than $(-1)^m d_1 d_2 \cdots d_m$, and as a consequence $d-1$ is bigger than $-d_m$. Finally, by the definition of m, the total number of shortest non-backtracking walks starting at i that self-intersect is $d(d-1)^m - (-1)^m d_1 d_2 \cdots d_m$. □

Theorem 95 shows that for every vertex i in a regular graph G, the path continued fraction for $\alpha_i(G)$ determines the length and total number of shortest non-backtracking walks starting at i that self-intersect.

As a corollary of Theorem 95, there is equality for regular graphs in the bound of Theorem 92 at least up to the girth, i.e., the length of the minimal cycle. The girth of the Petersen graph is 5, so Theorem 95 explains why there is equality up to 5 in the Table 4.2.

Theorem 96. *Consider the path continued fraction of* $\dfrac{\mu(G)'}{\mu(G)}$ *for a regular graph G with vertex weights x and edge weights* -1*. Then,* $-d_1$ *is equal to the degree of every vertex in G, and, if g is the largest index such that* $-d_2, \ldots, -d_{g-1}$ *are all equal to* $-(d_1 - 1)$*, then g is the girth of G and,*

$$(-1)^k n d_1 d_2 \cdots d_k = |\{c \in [\cdot \to \cdot] \mid l(c) = k\}|,$$

for every k in $[g]$*. In particular,* $nd(d-1)^{g-1} - (-1)^g n d_1 d_2 \cdots d_g$ *is equal to the total number of minimal directed cycles in G.*

Proof. The proof is analogous to that of Theorem 95, but using the path continued fraction of the logarithmic derivative of a matching polynomial. For the last part of the statement notice that the total number of shortest non-backtracking walks that self-intersect is precisely equal to the total number of minimal directed cycles in G. □

The Theorem 96 shows that the matching polynomial of a regular graph determines its degree, girth and total number of minimal cycles. This is one of the main results of the article by Beezer and Farrell [13, p. 12, Cor. 3.1].

In 2020, at the University of Waterloo's weekly seminar on Algebraic Graph Theory, Godsil posed the following question.

Question 97 (Godsil)**.** *Let G be a connected graph with vertex weights x and edge weights* -1 *such that* $\mu(G \setminus i)$ *equals* $\mu(G \setminus j)$ *for every pair of vertices i and j. Then, is G vertex-transitive?*

As a corollary of Theorems 95 and 96 we show a strong condition on graphs satisfying the hypothesis of Question 97. The result stated in the next corollary seems to be new.

Corollary 98. *Let G be a connected graph with girth g, vertex weights x and edge weights* -1*. If* $\alpha_i(G)$ *equals* $\alpha_j(G)$ *for every pair of vertices i and j, then* $\mu(G)$ *has distinct zeros and G is a regular graph such that every vertex is in a same number of cycles of length g.*

Proof. First, observe that the same proof of Theorem 45 implies that $\mu(G)$ has distinct zeros.

Let i be a vertex in the graph G and consider the path continued fraction for $\alpha_i(G)$. By Theorem 90 it follows that $-d_1$ is equal to the degree of i. Then, since all the graph continued fractions are equal, it follows that all vertices have the same degree and so G is a regular graph.

Now, since G is a regular graph, the Theorem 95 applies. Let m be the largest index such that $-d_2, \ldots, -d_{m-2}$ are all equal to $-(d_1 - 1)$. Then, Theorem 95 implies that,

$$(-1)^k d_1 d_2 \cdots d_k = |\{c \in [i \to \cdot] \mid l(c) = k\}|,$$

for every vertex i of G and every k in $[m]$. Theorem 96 together with Lemma 25 implies that m is actually equal to g.

If a vertex i is in a minimal cycle of G of length g, it then follows that the total number of minimal cycles containing i is, $\frac{1}{2}(d(d-1)^{g-1} - (-1)^g d_1 d_2 \dots d_g)$, which is independent of i.

If the vertex i were not in a minimal cycle, then, by the equality above, there would be a non-backtracking walk of length g starting at i that self-intersects at a vertex different from i. But this would necessarily produce a cycle that has length strictly smaller than g, which is impossible. This shows that every vertex is in a minimal cycle. □

4.3.3 Graph Continued Fractions for Locally-Finite Vertex-Transitive Graphs

A graph, possibly infinite, is named *locally-finite* if every vertex has finite degree. The study of graph continued fractions for locally-finite graphs has recently appeared in the literature with the works of Abért, Csikvari and Hubai [27] and Bordenave, Lelarge and Salez [19] in *matching measures* and by Bencs and Mészáros [15] in versions of the Gallai-Edmonds Theorem B.

The formulas for path continued fractions in Theorem 90 also apply to locally-finite graphs. This is the case because for a vertex i in a graph G, the coefficients with index smaller than k of the path continued fraction of $\alpha_i(G)$ depend only on the k-neighborhood of the vertex i. For this same reason, the graph continued fraction of a locally-finite rooted graph can be approximated by the graph continued fractions of a sequence of rooted graphs converging to it.

There is also a general continuous version for infinite graphs of the formulas in Theorem 84, similar to the equations in Section 4.1, which can be obtained using the Andreief-Heine identity [45, p. 2, Eq. 1.7] in place of the Cauchy-Binet formula of Proposition 82.

For a locally-finite vertex-transitive graph G with vertex weights x and edge weights -1, its *matching measure*, as defined in [27, p. 1, Def'n 1.1], is the unique measure with Stieltjes transform equal to $\frac{1}{\alpha_i(G)}$, for some vertex i of G. This measure is unique because it has bounded support by Theorem 28, and thus satisfies the solution of the moment problem mentioned in Section 4.1. As a consequence, the matching measure and the graph continued fraction of a locally-finite vertex-transitive graph carry essentially the same information.

In the article [27, p. 3] the authors note that there is some hope that for a locally-finite vertex-transitive graph its matching measure may reveal some interesting information about it.

In this section, we show that Theorem 92 extends to the setting of locally-finite vertex-transitive graphs and leads to an inequality involving its *connective constant* and the coefficients of the path continued fraction of its matching measure.

The connective constant of a locally-finite vertex-transitive graph is a quantity that encapsulates the growth of its self-avoiding walks. For a locally-finite vertex-transitive graph G with root i, denote by p_n the number of self-avoiding walks of length n starting at i. Since a self-avoiding walk of length $n+m$ can be broken in two self-avoiding walks of lengths n and m, it follows that $p_{n+m} \leq p_n p_m$. As a consequence, the limit $\mu_G := \lim_n p_n^{\frac{1}{n}}$ exists and is called the connective constant of G.

Self-avoiding walks and connective constants are an active topic of research. For more information about them see Madras and Slade's book [84] and the survey article by Bauerschmidt, Duminil-Copin, Goodman and Slade [12].

The next theorem presents an inequality connecting the path continued fraction associated with the matching measure and the connective constant of a locally-finite vertex-transitive graph.

Theorem 99. *Let G be a locally-finite vertex-transitive graph. Consider the path continued fraction of $\alpha_i(G)$ for some vertex i in G. Then, $(-1)^k d_1 d_2 \cdots d_k$ is bigger than, or equal to, p_k for every natural number k. As a consequence, $\liminf_k ((-1)^k d_1 d_2 \cdots d_k)^{\frac{1}{k}}$ is bigger than, or equal to, the connective constant of G.*

Proof. This is an immediate consequence of Theorem 92. □

In the next two examples, we examine the bounds of Theorem 99 for the square and hexagonal lattices. The path continued fractions for both lattices were calculated using the formulas of Section 4.1 and the number of tree-like walks of length smaller than 49 of both lattices, which are available in [21, p. 4, Table 1] and [27, p. 15]. The number of self-avoiding walks for the next examples was taken from [84, p. 394, Table C.1] and [83, p. 1433, Table 2].

Example 100 (Square lattice)**.** *Consider the path continued fraction associated with the matching measure of the square lattice. In Table 4.3 we present the approximate value of $-d_k$ in comparison with $\frac{p_k}{p_{k-1}}$ to* 3 *decimal places. This table already shows that the product $(-1)^k d_1 d_2 \cdots d_k$ is a lot larger than p_k. The connective constant of the square lattice satisfies the rigorous bounds,* $2.625622 \leq \mu_{\mathbb{Z}^2} \leq 2.679193$, *as can be seen in* [12, p. 4, Eq. 1.14].

Table 4.3: Comparison between $-d_k$ and $\frac{p_k}{p_{k-1}}$ for the square lattice.

k	1	2	3	4	5	6	7	8	9	10	11
$-d_k$	4	3	3	2.777	2.902	2.771	2.884	2.760	2.876	2.765	2.858
$\frac{p_k}{p_{k-1}}$	4	3	3	2.777	2.840	2.746	2.784	2.723	2.749	2.710	2.727

Since the square lattice can be well approximated by the cartesian products $C_n \times C_n$ with n large, where C_n is the cycle graph with n vertices, the values of Table 4.3 apply for these graphs as well.

Example 101 (Hexagonal lattice)**.** *Consider the path continued fraction associated with the matching measure of the hexagonal lattice. In Table 4.4 we present the* *approximate value of* $-d_k$ *in comparison with* $\dfrac{p_k}{p_{k-1}}$ *to* 3 *decimal places. This table shows that the product* $(-1)^k d_1 d_2 \cdots d_k$ *is also a lot larger than* p_k *in this case. The connective constant of the hexagonal lattice is known to be exactly* $\sqrt{2+\sqrt{2}} = 1.84775\ldots$*, by the work of Duminil-Copin and Smirnov* [34].

Table 4.4: Comparison between $-d_k$ and $\dfrac{p_k}{p_{k-1}}$ for the hexagonal lattice.

k	1	2	3	4	5	6	7	8	9	10	11	12	13
$-d_k$	3	2	2	2	2	1.875	1.991	1.957	1.950	1.896	2.011	1.912	1.940
$\dfrac{p_k}{p_{k-1}}$	3	2	2	2	2	1.875	1.933	1.931	1.928	1.879	1.911	1.896	1.899

The information presented in Examples 100 and 101 leads to the following question.

Question 102. *Let* G *be the square or hexagonal lattice and consider the path continued fraction of* $\alpha_i(G)$ *for some vertex* i *in* G*. Then, is it true that* $\liminf_k ((-1)^k d_1 d_2 \cdots d_k)^{\frac{1}{k}}$ *is strictly larger than the connective constant of* G*?*

In the article by Bencs and Mészáros [15, p. 36-37] there are other questions about the matching measure of lattices.

Chapter 5

Means of Near Continued Fractions

In this chapter, we shift focus and use the techniques presented in Section 2.3 to provide a different perspective on results in the classical theory of continued fractions and Pell's equation. In particular, we present a factoring algorithm that uses only the continued fraction of the square root of a natural number.

Classic continued fractions will be denoted by,

$$[a_0, a_1, a_2, \ldots, a_j, \ldots] := a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\ddots + \cfrac{1}{a_j + \cdots}}}}.$$

Two finite continued fractions are said to be *near* if one of them has one more term than the other. A pair of near continued fractions is represented by $[a_0, a_1, \ldots, a_k]$ and $[a_0, a_1, \ldots, a_k, a_{k+1}]$. In particular, two consecutive convergents of an irrational number are near continued fractions.

Our main theorem in this chapter provides formulas for the *arithmetic, geometric, harmonic* and *cotangent* means of near continued fractions. This theorem must certainly be known, but unfortunately we do not find it in the literature and we do not know who was the first to prove it.

Theorem 103 (Means of near continued fractions)**.** *Given $a_0, a_1, \ldots, a_{k+1}$ positive real numbers, it follows that,*

$$\frac{[a_0, a_1, \ldots, a_k] + [a_0, a_1, \ldots, a_k, a_{k+1}]}{2} = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1],$$

$$\sqrt{[a_0, a_1, \ldots, a_k] \cdot [a_0, a_1, \ldots, a_k, a_{k+1}]} = [a_0, \overline{a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, 2a_0}],$$

$$\frac{2}{\frac{1}{[a_0, a_1, \ldots, a_k]} + \frac{1}{[a_0, a_1, \ldots, a_k, a_{k+1}]}} = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0],$$

$$\cot\left(\frac{\cot^{-1}[a_0, a_1, \ldots, a_k] + \cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1}]}{2}\right) =$$

$$= [\overline{a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0}].$$

A complex version of Theorem 103 is also available.

Theorem 104 (Means of near complex continued fractions)**.** *Given* $a_0, a_1, \ldots, a_{k+1}$ *positive real numbers, it follows that,*

$$\frac{[a_0, a_1, \ldots, a_k, a_{k+1} - i] + [a_0, a_1, \ldots, a_k, a_{k+1} + i]}{2} =$$

$$= [a_0, a_1, \ldots, a_k, a_{k+1}, a_{k+1}, a_k, \ldots, a_1],$$

$$\sqrt{[a_0, a_1, \ldots, a_k, a_{k+1} - i] \cdot [a_0, a_1, \ldots, a_k, a_{k+1} + i]} =$$

$$= [a_0, \overline{a_1, \ldots, a_k, a_{k+1}, a_{k+1}, a_k, \ldots, a_1, 2a_0}],$$

$$\frac{2}{\dfrac{1}{[a_0, a_1, \ldots, a_k, a_{k+1} - i]} + \dfrac{1}{[a_0, a_1, \ldots, a_k, a_{k+1} + i]}} =$$

$$= [a_0, a_1, \ldots, a_k, a_{k+1}, a_{k+1}, a_k, \ldots, a_1, a_0],$$

$$\cot\left(\frac{\cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1} - i] + \cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1} + i]}{2}\right) =$$

$$= [\overline{a_0, a_1, \ldots, a_k, a_{k+1}, a_{k+1}, a_k, \ldots, a_1, a_0}].$$

Both theorems are proved using only algebraic manipulations of continuant polynomials, which are the numerators and denominators of classical continued fractions, and matching polynomials of paths. The condition of the positive numbers in both statements is to ensure convergence and that the objects are well defined, but the results apply to other types of continued fraction entries and notions of convergence.

The Theorem 103 should also be compared to the results of the work of Van der Poorten and Shallit [31, p. 239, Prop. 2] and [30, p. 604, Prop. 3]. These articles present a result analogous to the Arithmetic Mean formula with some signs changed, which is useful to transform some series into continued fractions.

In this section denote by $K[a_0, a_1, \ldots, a_n]$ the matching polynomial of the path with $n+1$ vertices with weights $a_0, \ldots, a_n$, respectively, and edge weights all equal to 1. Observe that,

$$[a_0, a_1, \ldots, a_n] = \frac{K[a_0, a_1, \ldots, a_n]}{K[a_1, \ldots, a_n]}, \quad \forall n \in \mathbb{N}\,.$$

In this setting, the Christoffel-Darboux Lemma 18 admits a particularly simple form.

Lemma 105 (Christoffel-Darboux for continuant polynomials)**.** *For every* $a_0, \ldots, a_n$*, it holds,*

$$K[a_0, a_1, \ldots, a_n]\cdot K[a_1, \ldots, a_n, a_{n+1}] - K[a_1, \ldots, a_n]\cdot K[a_0, a_1, \ldots, a_n, a_{n+1}] = (-1)^{n+1}.$$

The next lemma uses the recurrences of matching polynomials presented in Lemma 11 for the particular case of continuants.

Lemma 106 (Properties of symmetric continuants)**.** *For every* $a_0, a_1, \ldots, a_{k+1}$*, it holds:*

a) $K[a_0, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_0] = 2 \cdot K[a_0, \ldots, a_k] \cdot K[a_0, \ldots, a_k, a_{k+1}]$;

b) $K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1] =$
$= K[a_0, \ldots, a_k] \cdot K[a_1, \ldots, a_{k+1}] + K[a_0, \ldots, a_{k+1}] \cdot K[a_1, \ldots, a_k]$;

c) $K[a_0, \ldots, a_{k+1}, a_{k+1}, \ldots, a_0] =$
$= K[a_0, \ldots, a_{k+1}]^2 + K[a_0, \ldots, a_k]^2 =$
$= K[a_0, \ldots, a_k, a_{k+1} - i] \cdot K[a_0, \ldots, a_k, a_{k+1} + i]$;

d) $K[a_0, a_1, \ldots, a_{k+1}, a_{k+1}, \ldots, a_1] =$
$= K[a_0, \ldots, a_{k+1}] \cdot K[a_1, \ldots, a_{k+1}] + K[a_0, \ldots, a_k] \cdot K[a_1, \ldots, a_k]$.

Proof. a) A generalization of this item can be easily proved using graph continued fractions, as shown in Figure 5.1.

b) $K[a_0, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1] =$
$= 2a_{k+1} \cdot K[a_0, \ldots, a_k] \cdot K[a_1, \ldots, a_k] + K[a_0, \ldots, a_{k-1}] \cdot K[a_1, \ldots, a_k]+$
$K[a_0, \ldots, a_k] \cdot K[a_1, \ldots, a_{k-1}] =$
$= K[a_0, \ldots, a_k] \cdot (a_{k+1} \cdot K[a_1, \ldots, a_k] + K[a_1, \ldots, a_{k-1}])+$
$K[a_1, \ldots, a_k] \cdot (a_{k+1} \cdot K[a_0, \ldots, a_k] + K[a_0, \ldots, a_{k-1}]) =$
$= K[a_0, \ldots, a_k] \cdot K[a_1, \ldots, a_{k+1}] + K[a_0, \ldots, a_{k+1}] \cdot K[a_1, \ldots, a_k]$.

c) Conditioning at the edge connected to the two vertices weighted a_{k+1} implies: $K[a_0, \ldots, a_{k+1}, a_{k+1}, \ldots, a_0] = K[a_0, \ldots, a_{k+1}]^2 + K[a_0, \ldots, a_k]^2$.

Now, notice that, $K[a_0, \ldots, a_{k+1}]^2 + K[a_0, \ldots, a_k]^2 =$
$= (K[a_0, \ldots, a_{k+1}] - i \cdot K[a_0, \ldots, a_k])(K[a_0, \ldots, a_{k+1}] + i \cdot K[a_0, \ldots, a_k]) =$
$= K[a_0, \ldots, a_k, a_{k+1} - i] \cdot K[a_0, \ldots, a_k, a_{k+1} + i]$.

d) Once again, conditioning at the edge connected to the two vertices weighted a_{k+1} this item immediately follows. □

Theorems 103 and 104 are immediate consequences of Lemmas 105 and 106.

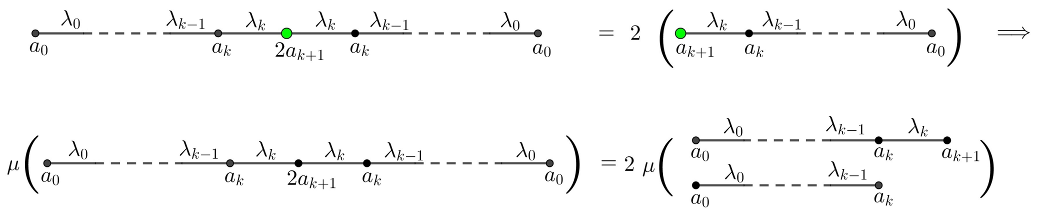


Figure 5.1: Proof of the item (a) of Lemma 106 using graph continued fractions. The first equality is a simple statement about continued fractions. After clearing the denominators, the second equality is obtained.

Proof of Theorems 103 and 104. We prove the formulas for all the means in Theorem 103. The proof of Theorem 104 is analogous and uses other properties of continuants listed in Lemma 106.

Arithmetic Mean:

$$\frac{[a_0, a_1, \ldots, a_k] + [a_0, a_1, \ldots, a_k, a_{k+1}]}{2} = \frac{\dfrac{K[a_0, a_1, \ldots, a_k]}{K[a_1, \ldots, a_k]} + \dfrac{K[a_0, a_1, \ldots, a_{k+1}]}{K[a_1, \ldots, a_{k+1}]}}{2} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_{k+1}] + K[a_0, a_1, \ldots, a_{k+1}] \cdot K[a_1, \ldots, a_k]}{2 \cdot K[a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_{k+1}]} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]} = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1].$$

Geometric Mean:

Consider $x = [a_0, \overline{a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, 2a_0}]$, we need to prove that,

$$x = \sqrt{[a_0, a_1, \ldots, a_k] \cdot [a_0, a_1, \ldots, a_k, a_{k+1}]}.$$

Note that,

$$x = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0 + x] =$$

$$= \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0 + x]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0 + x]} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1] \cdot x + K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1] \cdot x + K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0]} \implies$$

$$K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]x^2 = K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0] \implies$$

$$x = \sqrt{\frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]}} =$$

$$= \sqrt{\frac{2 \cdot K[a_0, a_1 \ldots, a_k] \cdot K[a_0, a_1, \ldots, a_k, a_{k+1}]}{2 \cdot K[a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_k, a_{k+1}]}} =$$

$$= \sqrt{[a_0, a_1, \ldots, a_k] \cdot [a_0, a_1, \ldots, a_k, a_{k+1}]}.$$

Harmonic Mean: Observe that,

$$\frac{2}{\frac{1}{[a_0, a_1, \ldots, a_k]} + \frac{1}{[a_0, a_1, \ldots, a_k, a_{k+1}]}} = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0] \iff$$

$$\frac{[0, a_0, a_1, \ldots, a_k] + [0, a_0, a_1, \ldots, a_k, a_{k+1}]}{2} = [0, a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0],$$

which is true by the formula for the Arithmetic Mean.

Cotangent Mean:

Consider $x := [\overline{a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0}]$, we need to prove that,

$$x = \cot\left(\frac{\cot^{-1}[a_0, a_1, \ldots, a_k] + \cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1}]}{2}\right).$$

Note that,

$$x = [a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0, x] =$$

$$= \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0, x]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0, x]} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0] \cdot x + K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0] \cdot x + K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]} \implies$$

$$\frac{x^2 - 1}{2x} = \frac{K[a_0, a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0] - K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1]}{2 \cdot K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0]} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k] \cdot K[a_0, a_1, \ldots, a_k, a_{k+1}] - K[a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_k, a_{k+1}]}{K[a_1, \ldots, a_k, 2a_{k+1}, a_k, \ldots, a_1, a_0]} =$$

$$= \frac{K[a_0, a_1, \ldots, a_k] \cdot K[a_0, a_1, \ldots, a_k, a_{k+1}] - K[a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_k, a_{k+1}]}{K[a_0, a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_k, a_{k+1}] + K[a_0, a_1, \ldots, a_k, a_{k+1}] \cdot K[a_1, \ldots, a_k]} =$$

$$= \frac{[a_0, a_1, \ldots, a_k] \cdot [a_0, a_1, \ldots, a_k, a_{k+1}] - 1}{[a_0, a_1, \ldots, a_k] + [a_0, a_1, \ldots, a_k, a_{k+1}]} \implies$$

$$\frac{x^2 - 1}{2x} = \frac{[a_0, a_1, \ldots, a_k] \cdot [a_0, a_1, \ldots, a_k, a_{k+1}] - 1}{[a_0, a_1, \ldots, a_k] + [a_0, a_1, \ldots, a_k, a_{k+1}]}.$$

Using this last equation and the formula for the cotangent of the sum:

$$\cot(y + z) = \frac{\cot y \cdot \cot z - 1}{\cot y + \cot z},$$

we obtain,

$$2 \cot^{-1} x = \cot^{-1}[a_0, a_1, \ldots, a_k] + \cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1}] \iff$$

$$x = \cot\left(\frac{\cot^{-1}[a_0, a_1, \ldots, a_k] + \cot^{-1}[a_0, a_1, \ldots, a_k, a_{k+1}]}{2}\right).$$

□

The Theorem 103 can be generalized to the case of graph continued fractions using the same idea that is presented in Figure 2.5 to obtain a formula for periodic continued fractions. In this way, formulas are obtained for the means of $\alpha_i(G)$ and $\alpha_i(G \setminus j)$.

5.1 Pell Equation and Factorization

For $\frac{p}{q} \in \mathbb{Q}_{>1}$ which is not a square in $\mathbb{Q}$, it is well known that,

$$\sqrt{\frac{p}{q}} = [a_0/2, \overline{a_1, a_2, \ldots, a_2, a_1, a_0}],$$

$$\frac{1 + \sqrt{\frac{p}{q}}}{2} = [(1 + b_0)/2, \overline{b_1, b_2, \ldots, b_2, b_1, b_0}],$$

with a_j and b_j natural numbers for every j, a_0 even and b_0 odd, where the central words, $(a_1, a_2, \ldots, a_2, a_1)$ and $(b_1, b_2, \ldots, b_2, b_1)$, are palindromes. Assume from now on that the periods of these continued fractions are minimal. For natural numbers these continued fraction expansions are of particular interest, as they give rise to the fundamental solutions of the Pell equation. If $\frac{p}{q}$ is equal to a natural number n, then,

$$K[a_0/2, a_1, a_2, \ldots, a_2, a_1]^2 - n \cdot K[a_1, a_2, \ldots, a_2, a_1]^2 = (-1)^l,$$

$$(2 \cdot K[b_0/2, b_1, b_2, \ldots, b_2, b_1])^2 - n \cdot K[b_1, b_2, \ldots, b_2, b_1]^2 = 4(-1)^m,$$

where l and m are the period lengths of the continued fractions expansions of $\sqrt{n}$ and $\frac{1+\sqrt{n}}{2}$, respectively.

In this case, l is odd if, and only if, the equation $x^2 - ny^2 = -1$ is solvable. If n is divisible by a prime p congruent to 3 modulo 4, then this last equation is unsolvable, because -1 is not an square modulo p. It follows that l is even whenever n is divisible by a prime congruent to 3 modulo 4. A similar reasoning applies for the parity of m.

Observe that,

$$\sqrt{n} = [a_0/2, \overline{a_1, a_2, \ldots, a_k, a_k, \ldots, a_2, a_1, a_0}],$$

if $l = 2k+1$ is odd, and,

$$\sqrt{n} = [a_0/2, \overline{a_1, a_2, \ldots, a_k, a_{k+1}, a_k, \ldots, a_2, a_1, a_0}],$$

if $l = 2k+2$ is even.

In this second case, one can apply the formula for the geometric mean of near continued fractions in Theorem 103 to obtain,

$$\sqrt{n} = \sqrt{[a_0/2, a_1, \ldots, a_k] \cdot [a_0/2, a_1, \ldots, a_k, a_{k+1}/2]} \iff$$

$$n = [a_0/2, a_1, \ldots, a_k] \cdot [a_0/2, a_1, \ldots, a_k, a_{k+1}/2].$$

In the case a_{k+1} is even, it then follows that n can be factored as the product of two near continued fractions with natural numbers as entries. This procedure is clearly reversible, as one can go from such a factorization to the continued fraction expansion of $\sqrt{n}$ using the geometric mean formula in Theorem 103.

Since both $K[a_0/2, a_1, \ldots, a_k]$ and $K[a_1, \ldots, a_k]$, and $K[a_0/2, a_1, \ldots, a_k, a_{k+1}/2]$ and $K[a_1, \ldots, a_k, a_{k+1}/2]$ are pairs of co-prime natural numbers, it follows that n can be factored as the product of two natural numbers as,

$$n = \frac{K[a_0/2, a_1, \ldots, a_k]}{K[a_1, \ldots, a_k, a_{k+1}/2]} \cdot \frac{K[a_0/2, a_1, \ldots, a_k, a_{k+1}/2]}{K[a_1, \ldots, a_k]}.$$

This factorization is non-trivial. Indeed, if this were not the case, then,

$$K[a_0/2, a_1, \ldots, a_k] = K[a_1, \ldots, a_k, a_{k+1}/2],$$

and from item f) in Lemma 105,

$$K[a_0/2, a_1, \ldots, a_k] \cdot K[a_1, \ldots, a_k, a_{k+1}/2] -$$

$$K[a_1, \ldots, a_k] \cdot K[a_0/2, a_1, \ldots, a_k, a_{k+1}/2] = (-1)^{k+1}.$$

As a consequence,

$$K[a_0/2, a_1, \ldots, a_k]^2 - n \cdot K[a_1, \ldots, a_k]^2 = (-1)^{k+1},$$

is a nontrivial solution for the Pell equation of n that is smaller than the fundamental solution, which is impossible.

The two non-trivial factors of the natural number n obtained this way are also co-prime because $K[a_0/2, a_1, \ldots, a_k]$ and $K[a_0/2, a_1, \ldots, a_k, a_{k+1}/2]$ are co-prime.

In conclusion, from the continued fraction of $\sqrt{n}$ it is sometimes possible to obtain a non-trivial factorization of n as the product of two co-prime naturals. This procedure, which appears to be new, is shown in practice in the next example.

Example 107.

$$\sqrt{741} = [27, \overline{4, 1, 1, 13, 18, 13, 1, 1, 4, 54}] = \sqrt{[27, 4, 1, 1, 13] \cdot [27, 4, 1, 1, 13, 9]} =$$

$$= \sqrt{\frac{3321}{122} \cdot \frac{30134}{1107}} = \sqrt{\frac{3321}{1107} \cdot \frac{30134}{122}} = \sqrt{3 \cdot 247} \implies 741 = 3 \cdot 247.$$

A similar observation appeared in the work of van der Poorten and Walsh [32, p. 52, Thm. 1], where they also mention a connection to the *lagrange equation.* The advantage of our approach is that the geometric mean formula of Theorem 103 holds under more general conditions and immediately shows that there exists a factorization.

In the way described above this factoring algorithm is slow in general because the period length of the continued fraction of $\sqrt{n}$ can be large. Using the theory of quadratic forms it is possible to obtain a faster algorithm, as presented in the work of Elia [36, p. 5-7].

If the period length of the continued fraction of $\sqrt{n}$ is odd, then it was already known by Legendre [79, p. 59-60] that one can obtain a primitive sum of squares representation of n. This fact can also be proved using the geometric mean formula in Theorem 104.

It is also possible, using Theorems 103 and 104, to give simplified proofs of some other results about the Pell and Lagrange equations and continued fractions of square roots.

5.2 Mordell's Conjecture

In this section, we study, using the procedure of Section 5.1, the continued fraction of $\sqrt{p^{2m-1}}$, where p is a prime congruent to 3 modulo 4 and m is a natural number. As a consequence, we obtain, following Chakraborty and Saikia [23], a restatement of a conjecture by Mordell [87].

First, notice that since p is congruent to 3 modulo 4 the period length of the continued fraction of $\sqrt{p^{2m-1}}$ is even. Write $\sqrt{p^{2m-1}} = [a_0/2, \overline{a_1, \ldots, a_k, a_{k+1}, a_k, \ldots, a_1, a_0}]$, where $a_0 = 2\lfloor\sqrt{p^{2m-1}}\rfloor$ is even, and the period is minimal.

Observe that a_{k+1} is odd, otherwise, by the procedure of Section 5.1, one can obtain a non-trivial factorization of p^{2m-1} as the product of two co-prime natural numbers, which is impossible.

Define,

$$s_{0,k+1} := 2 \cdot K[a_0/2, a_1, \ldots, a_k, a_{k+1}/2], \quad s_0 := K[a_0/2, a_1, \ldots, a_k],$$

$$s_{k+1} := 2 \cdot K[a_1, \ldots, a_k, a_{k+1}/2], \quad s := K[a_1, \ldots, a_k],$$

and observe that $s_{0,k+1}, s_0, s_{k+1}$ and s are natural numbers. By the geometric mean formula in Theorem 103 and Lemma 105, it holds that,

$$p^{2m-1} = \frac{s_0 \cdot s_{0,k+1}}{s \cdot s_{k+1}} = \frac{s_0}{s_{k+1}} \cdot \frac{s_{0,k+1}}{s}, \quad s_0 \cdot s_{k+1} - s \cdot s_{0,k+1} = 2(-1)^{k+1}.$$

We prove that $\frac{s_0}{s_{k+1}}$ and $\frac{s_{0,k+1}}{s}$ are co-prime natural numbers and $s_{0,k+1}, s_0, s_{k+1}$ and s are all odd.

Observe that by the second equation above it holds that both $\gcd(s_{0,k+1}, s_{k+1})$ and $\gcd(s_{0,k+1}, s_0)$ are equal to 1 or 2. It also follows from Lemma 105 that $\gcd(s_0, s) = 1$. Now, using the definition of continuant,

$$s_{0,k+1} = a_{k+1} \cdot s_0 + 2 \cdot K[a_0/2, a_1, \ldots, a_{k-1}], \quad s_{k+1} = a_{k+1} \cdot s + 2 \cdot K[a_1, \ldots, a_{k-1}],$$

from which follows, since a_{k+1} is odd, that both $s_{0,k+1}$ and s_0, and s_{k+1} and s are pairs of natural numbers with the same parity. Now, as $\gcd(s_0, s) = 1$, we get that the parity of the pair $s_{0,k+1}$ and s_0 is different from the parity of the pair s_{k+1} and s. It follows that $\gcd(s_{0,k+1}, s_{k+1}) = 1$. As a consequence, since both $\gcd(s_{0,k+1}, s_{k+1})$ and $\gcd(s_{0,k+1}, s_{k+1})$ are equal to 1 and the product $\frac{s_0}{s_{k+1}} \cdot \frac{s_{0,k+1}}{s}$ is a natural number, it follows that $\frac{s_0}{s_{k+1}}$ and $\frac{s_{0,k+1}}{s}$ are natural numbers and s_0 and s_{k+1} are odd.

Now, as $\gcd(s_{0,k+1}, s_0)$ is either 1 or 2, $s_{0,k+1}$ and s_0 have the same parity and the product $\frac{s_0}{s_{k+1}} \cdot \frac{s_{0,k+1}}{s}$ is odd, it follows that $\frac{s_0}{s_{k+1}}$ and $\frac{s_{0,k+1}}{s}$ are co-prime natural numbers and $s_{0,k+1}, s_0, s_{k+1}$ and s are all odd.

We also have $s \leq s_0, s_{k+1} < s_{0,k+1}$, from which follows $\frac{s_0}{s_{k+1}} < \frac{s_{0,k+1}}{s}$. Finally, we obtain,

$$\frac{s_0}{s_{k+1}} = 1, \quad \frac{s_{0,k+1}}{s} = p^{2m-1}.$$

By the geometric mean formula in Theorem 103 this implies,

$$\sqrt{p^{2m-1}} = \sqrt{\frac{s_{k+1}}{s_0} \cdot \frac{s_{0,k+1}}{s}} = \sqrt{\frac{s_{k+1}}{s} \cdot \frac{s_{0,k+1}}{s_0}} =$$

$$= 2\sqrt{[a_{k+1}/2, a_k, \ldots, a_1] \cdot [a_{k+1}/2, a_k, \ldots, a_1, a_0/2]} =$$

$$= 2 \cdot [a_{k+1}/2, \overline{a_k, \ldots, a_1, a_0, a_1, \ldots, a_k, a_{k+1}}] \implies$$

$$\frac{\sqrt{p^{2m-1}}}{2} = [a_{k+1}/2, \overline{a_k, \ldots, a_1, a_0, a_1, \ldots, a_k, a_{k+1}}] \iff$$

$$\frac{1+\sqrt{p^{2m-1}}}{2} = [(1+a_{k+1})/2, \overline{a_k, \ldots, a_1, a_0, a_1, \ldots, a_k, a_{k+1}}].$$

As a consequence, a_{k+1} is either $\lfloor \sqrt{p^{2m-1}} \rfloor$ or $\lfloor \sqrt{p^{2m-1}} \rfloor - 1$, whichever is odd.

Mordell's conjecture [87, p. 283] concerns a divisibility property of the fundamental solution of the Pell equation of p, where p is a prime congruent to 3 modulo 4. This conjecture was inspired by a similar conjecture of Ankeny, Artin and Chowla [4, p. 480], where p is a prime congruent to 1 modulo 4.

Conjecture 108 (Mordell [87])**.** *Let $x^2 - py^2 = 1$ be a fundamental solution of the Pell equation of p, where p is a prime congruent to* 3 *modulo* 4*. Then p does not divide y.*

This conjecture can be rewritten in the language of continued fractions. Write $\sqrt{p} = [a_0/2, \overline{a_1, \ldots, a_k, a_{k+1}, a_k, \ldots, a_1, a_0}]$, then Conjecture 108 is easily seen as equivalent to the statement that p does not divide $K[a_1, \ldots, a_k, a_{k+1}, a_k, \ldots, a_1]$.

In their work, Chakraborty and Saikia [23, p. 2551, Thm. 4.1] proved that Conjecture 108 is equivalent to the statement that p does not divide $K[a_1, \ldots, a_k]$. This is also a consequence of our results presented above.

First, observe that, by item (a) of Lemma 106, $K[a_1, \ldots, a_k, a_{k+1}, a_k, \ldots, a_1]$ equals $s_{k+1} \cdot s$. Notice that s is, by definition, equal to $K[a_1, \ldots, a_k]$. It suffices then to verify that s_{k+1} is not divisible by p. But $p = \dfrac{s_{0,k+1}}{s}$ and $\gcd(s_{0,k+1}, s_{k+1}) = 1$, so s_{k+1} is not divisible by p.

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