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Programa de Pós-Graduação em Matemática

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Exploring Quantum Walks: Weighted Paths and Quotient Graphs Unveiled

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Final Version

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FOLHA DE APROVAÇÃO

Exploring Quantum Walks: Weighted Paths and Quotient Graphs Unveiled

FREDERICO CANÇADO PEREIRA

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ATA DA DEFESA DE DISSERTAÇÃO DE MESTRADO DO ALUNO FREDERICO CANÇADO PEREIRA, REGULARMENTE MATRICULADO NO PROGRAMA DE PÓS-GRADUAÇÃO EM MATEMÁTICA DO INSTITUTO DE CIÊNCIAS EXATAS DA UNIVERSIDADE FEDERAL DE MINAS GERAIS, REALIZADA NO DIA 09 DE AGOSTO DE 2023.

Aos nove dias do mês de agosto de 2023, às 14h00, na sala 3060, reuniram-se os professores abaixo relacionados, formando a Comissão Examinadora homologada pelo Colegiado do Programa de Pós-Graduação em Matemática, para julgar a defesa de dissertação do aluno **Frederico Cançado Pereira**, intitulada: *"Exploring Quantum Walks: Weighted Paths and Quotient Graphs Unveiled"*, requisito final para obtenção do Grau de mestre em Matemática. Abrindo a sessão, o Senhor Presidente da Comissão, Prof. Gabriel de Morais Coutinho, após dar conhecimento aos presentes do teor das normas regulamentares do trabalho final, passou a palavra ao aluno para apresentação de seu trabalho. Seguiu-se a arguição pelos examinadores com a respectiva defesa do aluno. Após a defesa, os membros da banca examinadora reuniram-se reservadamente sem a presença do aluno e do público, para julgamento e expedição do resultado final. Foi atribuída a seguinte indicação: o aluno foi considerado aprovado sem ressalvas e por unanimidade. O resultado final foi comunicado publicamente ao aluno pelo Senhor Presidente da Comissão. Nada mais havendo a tratar, o Presidente encerrou a reunião e lavrou a presente Ata, que será assinada por todos os membros participantes da banca examinadora. Belo Horizonte, 09 de agosto de 2023.

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"*Freedom is the freedom to say that two plus two make four. If that is granted, all else follows.*"

(Orwell, George. 1984)

Resumo

Esta dissertação explora o problema da Transferência Perfeita de Estado (PST) em grafos, que tem implicações significativas na computação quântica. O objetivo é determinar quais grafos permitem transferir perfeitamente o estado de um qubit (ou vértice) para outro qubit em um determinado tempo. O texto apresenta uma introdução ao tema utilizando técnicas de álgebra linear, discutindo condições necessárias e suficientes para alcançar o PST e enfatizando a transferência de longa distância entre qubits. O objetivo da otimização é minimizar o número de componentes quânticos necessários para alcançar a transferência perfeita de estado.

Uma classe importante de grafos que admite PST são os caminhos com pesos. Para o PST entre vértices nos extremos, o problema foi completamente resolvido explorando a conexão desses grafos com polinômios ortogonais. No entanto, o problema se torna consideravelmente mais complexo para vértices em outras posições, levando a novos resultados e conexões explorados neste documento. Entre esses resultados, podemos citar uma fórmula que relaciona, de maneira inédita, o polinômio extremo com outro polinômio arbitrário em uma sequência de polinômios ortogonais; como criar uma sequência de polinômios ortogonais que contenha outros dois dados; e como o PST em caminhos com pesos se relaciona com o problema de Prouhet-Tarry-Escott, um problema em aberto na área de teoria dos números.

Por fim, o documento apresenta uma abordagem para a construção de grafos com PST, explorando caminhos ponderados e partições equitativas. Também são apresentados novos teoremas nessa área, que têm relevância geral para a teoria dos grafos. Entre esses teoremas, destaca-se um critério para dois grafos possuírem um quociente simetrizado em comum; como as matrizes de partições equitativas se relacionam com matrizes projetivas; e como o conjunto de partições equitativas se transforma quando o grafo original é quocientado.

Palavras-chave: Teoria espectral de grafos. Transferência perfeita de estado. Partição equitativa. Polinômios ortogonais.

Abstract

This thesis explores the problem of Perfect State Transfer (PST) in graphs, which has significant implications in quantum computing. The goal is to determine which graphs allow for perfect transfer of the state of one qubit (or vertex) to another qubit within a certain time frame. The text provides an introduction to the topic using techniques from linear algebra, discussing necessary and sufficient conditions to achieve PST, and emphasizing long-distance transfer between qubits. The optimization objective is to minimize the number of quantum components required to achieve perfect state transfer.

An important class of graphs that admit PST is weighted paths. For PST between vertices at the endpoints, the problem has been completely solved by exploring the connection of these graphs with orthogonal polynomials. However, the problem becomes considerably more complex for vertices in other positions, leading to new results and connections explored in this document. Among these results, we can mention a formula that uniquely relates the extreme polynomial to another arbitrary polynomial in a sequence of orthogonal polynomials, how to create a sequence of orthogonal polynomials containing two given polynomials, and how PST in weighted paths relates to the Prouhet-Tarry-Escott problem, an open problem in number theory.

Finally, the document presents an approach to constructing graphs with PST, exploring weighted paths and equitable partitions. New theorems in this are also presented, which have general relevance to graph theory. These theorems include a criterion for two graphs to have a common symmetrized quotient, how equitable partition matrices relate to projective matrices, and how the set of equitable partitions transforms when the original graph is quotiented.

Keywords: Spectral graph theory. Perfect state transfer. Equitable partition. Orthogonal polynomials.

Notation

- R: an arbitrary commutative ring;
- $R[t]$: the ring of polynomials with coefficients in R;
- $R[[t]]$: the ring of generating functions with coefficients in R;
- $\sigma(M) := \{\lambda \in R\colon \det(\lambda I - M) = 0\}$: the spectrum of $M \in \mathbb{M}_n(R)$;
- $S^1 := \{z \in \mathbb{C}; |z| = 1\}$: the unit circle in $\mathbb{C}$;
- $\mathbb{M}_{m,n}(R)$: the R-module of $m \times n$ matrices with entries in R;
- $\mathbb{M}_n(R) := \mathbb{M}_{n,n}(R)$;
- M^* denotes the adjoint of M: the matrix transposed and point-wise conjugated;
- M^T denotes the transpose of M;
- I_m or simply I: the identity $m \times m$ matrix;
- e_n: the vector with all entries 0, except the n^{th}, which is 1;
- χ_S: the characteristic vector of S, that is $\sum_{r\in S} e_r$;
- $\mathbb{1}$: the vector with all entries 1;
- J: the matrix with all entries 1;
- $\xi \parallel \zeta$: the vectors ξ and ζ are parallel;
- $(X)_R$: for $X \subseteq M$, where M is a R-module, the R-module generated by the elements of X. When $X = \{v_1, \ldots, v_n\}$, we shall use only $(v_1, \ldots, v_n)_R$, and we may omit the ring of scalars when it is clear; in particular, if $R = M$, $(X)_R$ is the ideal generated by X;
- $R[A]$: for $A \subseteq M$, where M in a R-algebra, this denotes the R-sub-algebra generated by A;
- $V(X)$: the set of vertices of the graph X;
- $E(X)$: the set of edges of the graph X;
- $d_X(a, b)$: the distance between the vertices a and b in the graph X;
- $N(a, V')$: for $a \in V(X)$ and $V' \subseteq V(X)$, the number of edges incident to a with the other vertex in V';
- $\operatorname{rng} f$: the range of the function f;
- $\Re z$ and $\Im z$: respectively, the real part and imaginary part of z;
- $\operatorname{res}(f(z); z = z_0)$: the residue of f at the point z_0.

Contents

Chapter 1

Introduction

1.1 Introduction to the problem

We can model a system of d qubits, which may or may not interact with each other, using a graph with d vertices. In this graph, an edge represents an interaction between two qubits.

In this system, the Hamiltonian, whose exponential describes the temporal evolution of the system, is given by the matrix:

$$H = \frac{1}{2} \sum_{ab \in E(X)} X_a X_b + Y_a Y_b,$$

where X_k corresponds to the operator that applies the Pauli matrix $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ to the qubit in position k, and similarly for Y_k and the Pauli matrix $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. The given Hamiltonian is a block matrix, and a detailed description and derivation using physical principles can be found in [3, 5, 7].

However, the block of the Hamiltonian matrix H that corresponds to the pure states of the qubits is determined by the adjacency matrix of the graph:

$$A_{a,b} = \begin{cases} 1 & a \sim b \\ 0 & a \nsim b \end{cases}.$$

Hence, a part of the quantum dynamics of the system can be described by the matrix exponential e^{itA}, as predicted by Schrödinger's equation. For more details, see [14, 20].

A problem of great interest, particularly in quantum computation, is the following: which graphs allow for a specific time at which the state of a given qubit (or vertex) a can be perfectly transferred to another qubit b?

If such a time exists, we say there is Perfect State Transfer (PST) between a and b (due to symmetry, we do not need to specify which vertex is the initial or the final). In

Chapter 3, we approach this question using solely linear algebra techniques. We discuss the necessary and sufficient conditions for achieving PST and explore various aspects of this phenomenon, based on [11, 18, 19].

Our particular interest lies in achieving PST between two vertices far apart in the graph. This capability would enable the transfer of qubit states between physically separated regions of a quantum computer without any loss of information.

An optimization goal that we aim to achieve is to utilize the fewest possible quantum components for transportation. In other words, we seek to construct a graph X with the minimum number of edges or vertices while still having PST between vertices separated by distance d. This problem is formalized and explored in Section 4.3. Within this section, we present known lower bounds and upper bounds related to this optimization problem.

Chapters 1, 2, and 3 provide a concise overview of the mathematical framework necessary to understand the phenomenon of PST, based mainly on [11]. In the remaining portion of this chapter, we will explore some critical well-known results in linear algebra. Chapter 2 focuses on general results in spectral graph theory, while Chapter 3 specifically addresses PST in graphs and introduces the main equivalence theorem, Theorem 3.10.

In Chapter 4, we delve into a discussion of graphs that exhibit PST, as well as important classes of graphs that do not. Furthermore, we explore methods for constructing new graphs with PST based on existing ones, based on [11, 21]. It is worth noting that the approach presented in this chapter may not be highly efficient, as it tends to increase the distance between vertices with PST linearly while exponentially increasing the number of vertices in the graph.

The remaining chapters, Chapter 5 and Chapter 6, introduce a novel approach to constructing graphs with PST. In Chapter 5, we focus on characterizing weighted paths that exhibit PST between their endpoints, a result attributed to [27]. Additionally, we present a new analysis of the necessary and sufficient conditions for achieving PST between an endpoint and an arbitrary vertex in a weighted path. In this chapter, we utilize the theory of orthogonal polynomials as a tool and develop new formulas and results to aid us in our objective.

In Chapter 6, our attention is devoted to the problem of constructing simple graphs with PST based on a given weighted graph that already possesses PST. To tackle this problem, we delve into the theory of equitable partitions. We explore results from [11, 21] and novel results. In this chapter, we not only prove new results that contribute to the general algebraic theory of graphs but also offer insights relevant to the study of PST.

1.2 Preliminary results

For the sake of self-containment, this section will encompass essential results and definitions from linear algebra that are not directly related to combinatorics or graphs but are crucial for understanding the thesis.

1.2.1 Matrices & self-adjointness

For a commutative ring R, we define the R-module $\mathbb{M}_{m,n}(R)$ as the set of $m \times n$ matrices with entries in R and point-wise sum and scalar multiplication. They are isomorphic to the R-module of R-linear functions that map R^n into R^m (again, with point-wise sum and scalar multiplication) by:

$$T \mapsto M_T := \Big(Te_1, Te_2, \dots, Te_n\Big),$$

which also satisfies $M_{S \circ T} = M_S M_T$ with the usual matrix product. In general, $\mathbb{M}_{m,n}(R) \cong R^{m \cdot n}$, as R-modules.

Our central case of interest will be when $R = \mathbb{C}$ or $R = \mathbb{R}$, despite having some matrices over $R[[t]]$ appearing in the text.

In the standard way, we can define the **norm** of a matrix as

$$\|M\| = \min_{v \neq 0} \frac{\|Mv\|}{\|v\|},$$

where $\|\cdot\|$ is the Euclidean norm.

Besides the normal matrix product, we also have two other types of products:

Definition 1.1. *Given two matrices $A, B \in \mathbb{M}_{m,n}(R)$ we define their* ***Schur product*** *as*

$$(A \circ B)_{a,b} := A_{a,b} B_{a,b},$$

or, in other words, the point-wise product of the matrices. The new matrix has dimension $m \times n$.

Definition 1.2. *Given two matrix $A \in \mathbb{M}_{m,n}(R), B \in \mathbb{M}_{p,q}(R)$, we define their* ***Kronecker product*** *as*

$$A \otimes B := \begin{pmatrix} a_{1,1}B & a_{1,2}B & \cdots & a_{1,n}B \\ a_{2,1}B & a_{2,2}B & \cdots & a_{2,n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1}B & a_{m,2}B & \cdots & a_{m,n}B \end{pmatrix}.$$

We also define the ***Kronecker sum*** *of these matrices by:*

$$A \oplus B := A \otimes I + I \otimes B.$$

Both operations define a matrix of dimension $mp \times nq$.

We list some properties of the three operations:

Proposition 1.3. *The following identities are valid whenever the matrix product is well-defined:*

(1) *The Schur product, Kronecker product, and Kronecker sum are associative and bilinear;*
(2) *The Schur product is commutative;*
(3) *The Kronecker product and sum are* ***not*** *commutative, however, given m, n, p, q we have permutations matrices P, Q such that $P(A \otimes B)Q = B \otimes A$ and $P(A \oplus B)Q = B \oplus A$ for every $A \in \mathbb{M}_{m,n}(R), B \in \mathbb{M}_{p,q}(R)$;*
(4) $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$;
(5) $(A \otimes B) \circ (C \otimes D) = (A \circ C) \otimes (B \circ D)$;
(6) $A \otimes B = (A \otimes I)(I \otimes B)$;
(7) $\sigma(A \otimes B) = \sigma(A) \cdot \sigma(B)$;
(8) $\sigma(A \oplus B) = \sigma(A) + \sigma(B)$;
(9) $\det(A \otimes B) = \det(A)^m \det(B)^n$*, where m, n are the size of A, B;*
(10) *A, B are both invertible iff $A \otimes B$ is, in that case $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$;*
(11) $(A \otimes B)^* = A^* \otimes B^*$;
(12) $(A \circ B)^* = A^* \circ B^*$;
(13) $\operatorname{tr}(A \otimes B) = (\operatorname{tr} A)(\operatorname{tr} B)$;
(14) $\operatorname{rk}(A \otimes B) = (\operatorname{rk} A)(\operatorname{rk} B)$;
(15) $e^{A \oplus B} = e^A \otimes e^B$;
(16) $\operatorname{rk}(A \circ B) \leq (\operatorname{rk} A)(\operatorname{rk} B)$;
(17) *If $A, B \geq 0$ then $A \circ B \geq 0$ and $\det(A \circ B) \geq \det A \det B$;*
(18) $(A \oplus B)^n = \sum_r \binom{n}{r} A^{n-r} \otimes B^r$.

There are some important classes of matrices defined on $\mathbb{M}_n(\mathbb{C})$: M is **self-adjoint** if $M^* = M$; M is called **normal** if $MM^* = M^*M$; M is **orthogonal** if $MM^* = I$; and M is **positive semidefinite** if $v^*Mv \geq 0$ for each v, in which case we denote $M \geq 0$, as well as, $M \geq N$ if $M - N \geq 0$.

The main theorem relating these concepts is:

Theorem 1.4 (Spectral theorem). *Let $M \in \mathbb{M}_n(\mathbb{C})$. Then, M is normal iff it is possible to write M as*

$$M = \sum_{r=1}^{d} \lambda_r E_r$$

where λ_r are the eigenvalues of M, d the number of distinct eigenvalues, and E_r satisfies:

(1) $E_r^2 = E_r$,

(2) $E_r = E_r^*$,

(3) $E_r E_s = 0$ *for all* $r \neq s$,

(4) $\sum E_r = I$.

They are the orthogonal projectors onto the eigenspaces of M, which are pair-wise orthogonal and sum to the whole space.

In this case, M is self-adjoint iff $\sigma(M) \subseteq \mathbb{R}$, M is orthogonal iff $\sigma(M) \subseteq S^1$, and $M \geq 0$ iff $\sigma(M) \subseteq [0, \infty)$.

We observe that as $\mathbb{M}_n(\mathbb{C})$ is a $\mathbb{C}$-algebra, it is possible to evaluate polynomials $p = \sum a_r t^r \in \mathbb{C}[t]$ over a matrix A, defined by $p(A) := \sum a_r A^r$. This application satisfies some properties:

Proposition 1.5 (Functional calculus). *The application*

$$\varphi_M \colon \mathbb{C}[t] \to \mathbb{M}_n(\mathbb{C})$$

$$p \mapsto p(A)$$

is a $\mathbb{C}$-algebra homomorphism. The range of φ_M is a subset of the matrices that commute with M, being all these matrices iff M is non-derogatory (that is, its minimal polynomial is equal to its characteristic polynomial).

Moreover, if $M = \sum \lambda_r E_r$ is normal we have:

$$p(M) = \sum p(\lambda_r) E_r.$$

In particular, $p(M)$ is normal. If M is invertible (which is equivalent to $0 \notin \sigma(M)$), we have

$$M^{-1} = \sum \lambda_r^{-1} E_r.$$

In the case where $f(z) = \sum a_r z^r$ is an entire function, we can define:

$$f(M) := \sum a_r M^r = \sum f(\lambda_r) E_r,$$

which satisfies the same properties.

This result gives us the following proposition:

Proposition 1.6. *Let X be a graph with adjacency matrix A. Then for each spectral projector E_j we have a polynomial $f \in \mathbb{C}[t]$ such that*

$$f(A) = E_j$$

Proof. Proposition 1.5 gives us $f(A) = \sum f(\lambda_r)E_r$. We can use Lagrange's interpolation to construct a polynomial of value 0 in each λ_r for $r \neq j$ and 1 in λ_j. □

We also have spectral knowledge on $p(M)$.

Theorem 1.7 (Spectral mapping theorem)**.** *For any $M \in \mathbb{M}_n(\mathbb{C})$ and $p \in \mathbb{C}[t]$ (or entire function) we have:*

$$\sigma(p(M)) = p(\sigma(M)),$$

$$\sigma(M^*) = \sigma(M)^*,$$

where $\sigma(M)^*$ denotes point-wise complex conjugation.

Another useful definition that will be related to connected graphs is

Definition 1.8. *We say that a non-negative matrix $M \in \mathbb{M}_n(\mathbb{R})$ is **irreducible** if there is no permutation P for which*

$$M = \begin{pmatrix} A & B \\ 0 & C \end{pmatrix},$$

where A and C are square matrices. Or, equivalently M is irreducible if for each a, b there is some r for which $(M^r)_{a,b} \neq 0$.

This is mainly used as a hypothesis for the next theorem. Perron and Frobenius independently proved it in [15, 23]. See [24] for a proof.

Theorem 1.9 (Perron-Frobenius)**.** *If M is non-negative and irreducible, then the eigenvector related to the largest absolute eigenvalue has only positive entries, is simple, and its eigenvalue is also positive.*

The number $\rho(M) := \max_{\lambda \in \sigma(M)} |\lambda|$ is called the spectral radius of M, and it is equivalent to $\|M\|$ when M is self-adjoint.

Chapter 2

Algebraic combinatorics

This chapter, as well as chapter 3 and 4, primarily draws upon [11, 16, 18, 19]. It is noteworthy that a comprehensive and refined elucidation of graph theory's nomenclature and fundamental principles can be found within [1, 18].

2.1 Spectral graph theory

We aim to see how to apply matrices and spectral theory in finite combinatorics, mostly graphs. Firstly, we have our primary definition:

Definition 2.1. *Let X be an arbitrary graph. We define the* ***adjacency matrix*** *$A(X)$, or simply A when it is clear, as the matrix with entries in $V(X)$ defined by*

$$A_{a,b} = \begin{cases} 1 & a \sim b \\ 0 & a \not\sim b \end{cases}.$$

We will start by relating the matrix A and its powers to the combinatorial properties of the graph. One of the most important combinatorial propositions is the following:

Proposition 2.2. *Let X be a graph. Then $(A^r)_{a,b}$ is the number of walks of length r from a to b in X.*

Proof. The proof is simple and follows by induction. For $r = 0$ (or 1), it is obvious. For the inductive step, we have:

$$(AA^r)_{a,b} = \sum_x A_{a,x}(A^r)_{x,b} = \sum_{x \sim b}(A^r)_{x,b}.$$

Thus, we are summing the number of r-walks from a to a vertex adjacent to b, which concludes the proof. □

Corollary 2.3. *For a graph X with adjacency matrix A, the distance between two vertices in the same connected component can be calculated by:*

$$d_X(a,b) = \min\{r; (A^r)_{a,b} \neq 0\}.$$

Corollary 2.4. *X is connected iff A is irreducible.*

With that in mind, we can define the generating function that counts walks in the graph, given by the formula

$$W(X,t) := \sum_r t^r A^r \in \mathbb{M}_n(\mathbb{C})[[t]].$$

We can verify by a direct multiplication that

$$W(X,t) = (I - tA)^{-1}.$$

Using the natural isomorphism $\mathbb{M}_n(\mathbb{C})[[t]] \cong \mathbb{M}_n(\mathbb{C}[[t]])$, given by

$$\varphi\colon \mathbb{M}_n(R)[[t]] \to \mathbb{M}_n(R[[t]]);$$

$$[t^n]\phi(f)_{a,b} = ([t^n]f)_{a,b};$$

$$\sum A_n t^n \mapsto \begin{pmatrix} \sum_n (A_n)_{1,1} t^n & \sum_n (A_n)_{1,2} t^n & \cdots & \sum_n (A_n)_{1,k} t^n \\ \sum_n (A_n)_{2,1} t^n & \sum_n (A_n)_{2,2} t^n & \cdots & \sum_n (A_n)_{2,k} t^n \\ \vdots & \vdots & \ddots & \vdots \\ \sum_n (A_n)_{k,1} t^n & \sum_n (A_n)_{k,2} t^n & \cdots & \sum_n (A_n)_{k,k} t^n \end{pmatrix},$$

we can make sense of expressions such as $\det(W(X,t)) \in \mathbb{C}[[t]]$ and $W_{a,b} \in \mathbb{C}[[t]]$.

We finally observe that A is self-adjoint, and we can use the spectral theorem (hence the name spectral graph theory).

It also follows from Proposition 1.5 that

Proposition 2.5.

$$W(X,t) = \sum \frac{1}{1 - t\lambda_r} E_r,$$

$$W(X,t)_{a,b} = \sum \frac{1}{1 - t\lambda_r} (E_r)_{a,b}.$$

Recall that the characteristic polynomial of a matrix is defined as follows:

$$\phi(X,t) := \det(tI - A) = \prod (t - \lambda_r)^{m_r},$$

where m_r is the multiplicity of λ_r. We have $m_r = \dim \operatorname{col} E_r = \operatorname{tr} E_r$. These calculations give us equality stated in the following proposition.

Proposition 2.6. *For a general graph, we have:*

$$\operatorname{tr}(W(X,t)) = \sum_r \frac{m_r}{1-t\lambda_r} = t^{-1}\frac{\phi'(X,t^{-1})}{\phi(X,t^{-1})}.$$

Proof. The first equality is already done. For the second, a direct differentiation gives us the following:

$$\phi'(X,t) = (\prod (t-\lambda_r)^{m_r})' = \sum_r m_r(t-\lambda_r)^{m_r-1}\prod_{s\neq r}(t-\lambda_s)^{m_r},$$

Thus,

$$\frac{\phi'(X,t)}{\phi(X,t)} = \sum_r \frac{m_r}{t-\lambda_r},$$

and a simple substitution $t \hookleftarrow t^{-1}$ allows us to conclude the result. □

By definition, $\operatorname{tr} W(X,t)$ is the generating function for the number of cycles in X, whence we were able to recover some combinatorial information simply from the characteristic polynomial $\phi(X,t)$. It is **not** possible to recover the whole graph X from its characteristic polynomial, for there are distinct graphs with the same polynomial. One example is the following pair of graphs, both of which have the same characteristic polynomial:

This example is not an isolated case. For instance, Schwenk showed that almost no tree is uniquely determined by its spectrum [26].

However, much information can be recovered from $\phi(X,t)$. For the next theorem, we shall make use of Lagrange's formula for determinant:

$$M \cdot \operatorname{adj}(M) = \det(M)I,$$

which works for $M \in \mathbb{M}_n(R)$ for *any* ring R. When $R = \mathbb{C}[[t]]$ and $M := (I - tA) = W(X,t)^{-1}$ we conclude that

$$W(X,t) = \frac{1}{\det(I-tA)}\operatorname{adj}(I-tA).$$

We observe that, by definition, $\operatorname{adj}(I-tA)_{a,a} = t\det((I-tA)[a,a])$, where $M[a,a]$ denotes the matrix M without the row and column a, which is equivalent to remove the vertex a from the graph. Thus by replacing $t \hookleftarrow t^{-1}$ we have:

Theorem 2.7. *Denoting by $X \setminus a$ the induced sub-graph obtained upon removing a from X, we have:*

$$t^{-1}W(X,t^{-1})_{a,a} = \frac{\phi(X \setminus a, t)}{\phi(X,t)},$$
$$\frac{\phi(X \setminus a, t)}{\phi(X,t)} = \sum_r \frac{(E_r)_{a,a}}{t-\lambda_r},$$
$$(E_r)_{a,a} = \left.\frac{\phi(X \setminus a, t)(x-\lambda_r)}{\phi(X,t)}\right|_{t=\lambda_r}.$$

Proof. The first equation can be derived from the previous observation. The second equation follows from Proposition 2.5, the first equation, and by performing the substitution $t \hookleftarrow t^{-1}$. The last equation is obtained by a direct substitution. □

We can utilize the characteristic polynomial to derive a formula for the off-diagonal entries of the adjacency matrix. However, this requires additional effort. To begin, we will start with some definitions.

Definition 2.8. *Let $a, b \in V(X)$. A* ***non-returning walk*** *from b to a is a walk from b to a that uses b only once. The generating function on non-returning walks from b to a is denoted by $N(X,t)_{b,a}$.*

An arbitrary n-walk from b to a consists of a non-returning walk from b to a of length j followed by a walk from a to a of length k, such that $k + j = n$. Thus, by the product convolution of generating functions, we have:

Proposition 2.9. *For $a, b \in V(X)$ distinct we have*

$$W(X,t)_{b,a} = W(X,t)_{a,a}N(X,t)_{b,a}.$$

Lemma 2.10. *For $a, b \in V(X)$ distinct we have*

$$W(X,t)_{a,a} - W(X \setminus b, t)_{a,a} = \frac{W(X,t)^2_{a,b}}{W(X,t)_{b,b}}.$$

Proof. A walk from a to a that uses the vertex b at least once can be decomposed uniquely as a walk that goes from a to b, followed by a non-returning walk from b to a. In terms of generating function, this gives us

$$W(X,t)_{a,a} - W(X \setminus b, t)_{a,a} = W(X,t)_{a,b}N(X,t)_{b,a},$$

and the result follows using that $W(X,t)$ is self-adjoint and the previous proposition. □

Now we are ready to demonstrate the off-diagonal formula:

Theorem 2.11. *For $a, b \in V(X)$ distinct vertices, we have*

$$t^{-1}W(X,t^{-1})_{a,b} = \frac{\sqrt{\phi(X\setminus a,t)\phi(X\setminus b,t) - \phi(X\setminus ab,t)\phi(X,t)}}{\phi(X,t)},$$

$$(E_r)_{a,b} = \left.\frac{(t-\lambda_r)\sqrt{\phi(X\setminus a,t)\phi(X\setminus b,t) - \phi(X\setminus ab,t)\phi(X,t)}}{\phi(X,t)}\right|_{t=\lambda_r};$$

where $X \setminus ab$ is the sub-graph induced in X by removing a, b.

Proof. By the previous lemma, we have

$$W(X,t)^2_{a,b} = W(X,t)_{a,a}W(X,t)_{b,b} - W(X\setminus b,t)_{a,a}W(X,t)_{b,b},$$

replacing $t \leftarrow t^{-1}$, multiplying both sides by t^{-1} and using Theorem 2.7 we conclude the first formula. The second follows from Proposition 2.5. □

2.2 Cospectrality

In this section, we present a relaxation on the condition of perfect state transfer. We shall define cospectrality as follows:

Definition 2.12. *Two vertices a, b of a graph X are said to be cospectral if for every $k \in \mathbb{N}$ the number of k-walks that start and end at a is equal to the number of k-walks that start and end at b.*

Now, we will define a tool that is useful for studying cospectrality and algebraic combinatorics in general:

Definition 2.13. *For a graph X with adjacency matrix A and a subset $S \subseteq V(X)$ we define the walk matrix relative to S as the matrix:*

$$W_S := \begin{pmatrix} \chi_S & A\chi_s & A^2\chi_S & \cdots & A^{n-1}\chi_S \end{pmatrix},$$

where χ_S is the characteristic vector of S.

We see that the columns of this matrix form a basis for the $\mathbb{R}[A]$-module generated by χ_S since $\phi(A) = 0$, which gives us that for some f with maximum degree $n-1$, $A^n = f(A)$. The walk modules on S help count the number of walks with vertices belonging to S.

Now we are ready to enunciate the following theorem:

Theorem 2.14. *For $a, b \in V(X)$ the following conditions are equivalent:*

(1) a, b are cospectral (that is $(A^k)_{a,a} = (A^k)_{b,b}$ for each k),

(2) $(E_r)_{a,a} = (E_r)_{b,b}$ for each d,

(3) $\phi(X \setminus a, t) = \phi(X \setminus b, t)$,

(4) $W_a^* W_a = W_b^* W_b$,

(5) the $\mathbb{R}[A]$-modules generated by $e_a + e_b$ and $e_a - e_b$ are orthogonal,

(6) there is a symmetric matrix $Q \in \mathbb{M}_n$ that commutes with A, $Q^2 = I$ and $Qe_a = e_b$,

(7) there is a orthogonal matrix $Q \in \mathbb{M}_n$ that commutes with A and $Qe_a = e_b$.

Proof. (1) and (2) are equivalent by Proposition 2.5, (2) and (3) are equivalent for the Theorem 2.7. For (4), we observe that

$$(W_a^* W_a)_{j,k} = e_a^* (A^{j-1})^* A^{k-1} e_a = (A^{k+j-2})_{a,a},$$

thus $(A^k)_{a,a} = (A^k)_{b,b}$ are equal for $0 \le k \le 2n-2$, but since A^k for $k \ge n$ is a linear combination of $I, A, ..., A^{n-1}$ we conclude that (4) is equivalent to (1).

For (5), we have

$$\begin{aligned}\langle A^k(e_a - e_b), A^j(e_a + e_b)\rangle &= (A^{k+j})_{a,a} - (A^{k+j})_{b,b} + (A^{k+j})_{a,b} - (A^{k+j})_{b,a} \\ &= (A^{k+j})_{a,a} - (A^{k+j})_{b,b},\end{aligned}$$

thus $A^k(e_a - e_b) \perp A^j(e_a + e_b)$ iff $(A^{k+j})_{a,a} = (A^{k+j})_{b,b}$ and the equivalence follows.

For (5) $\implies$ (6) we define Q as being the operator that is $-I$ on the $\mathbb{R}[A]$-module generated by $e_a - e_b$ and I on its orthogonal complement. $Q^2 = I$ and Q is symmetric. For an arbitrary $v \in \mathbb{R}^n$ we have $v = w_1 + w_2$ with w_1 in the module and w_2 in its complement; a simple calculation gives us that:

$$QA(w_1 + w_2) = Q(Aw_1 + Aw_2) = -Aw_1 + Aw_2 = AQ(w_1 + w_2),$$

where we used that the $\mathbb{R}[A]$-module and its complement are A-invariant. The last condition follows from (5)

$$Q(2e_a) = Q(e_a + e_b + e_a - e_b) = e_a + e_b - (e_a - e_b) = 2e_b.$$

It is clear that (6) $\implies$ (7) and for (7) $\implies$ (1) we have

$$\begin{aligned}e_b^* A^k b_a &= (Qe_a)^* A^k (Qe_a) \\ &= e_a^* Q^* A^k Q e_a \\ &= e_a^* Q^* Q A^k e_a \\ &= e_a^* A^k e_a;\end{aligned}$$

which concludes the proof. □

The condition (7) will also let us relate cospectrality with symmetries. First, we shall define the most apparent type of symmetry on graphs:

Definition 2.15. *A* ***graph isomorphism*** *between the graphs X and Y is a bijection $\varphi\colon V(X) \to V(Y)$, such that $\varphi(x) \sim \varphi(y) \iff x \sim y$. When $X = Y$, we say that φ is an automorphism.*

The automorphisms form a group with the composition operation, which is called the group of automorphisms of a graph, $\mathrm{Aut}(X)$. We observe that an X automorphism is, in particular, a permutation on $V(X)$. If there is an automorphism $\phi \in \mathrm{Aut}(X)$ such that $\phi(a) = b$, we say that the vertices a and b are **similar**.

A **permutation matrix**, related to the permutation σ, is a the linear transformation P such that $Pe_a = e_{\sigma(a)}$, that is, $P_{r,s} = 1$ if $\sigma(r) = s$ and zero otherwise. The following proposition relates permutation matrices and automorphisms:

Proposition 2.16. *A permutation on $V(X)$ is an X-automorphism iff its permutation matrix commutes with the adjacency matrix of X.*

Proof. It is easy to see that the following sentences are equivalent:

- P is automorphism;
- $P(a) \sim P(b) \iff a \sim b$;
- $e_a^* P^* A P e_b = 1 \iff A_{a,b} = 1$;
- $P^* A P = A$;
- $PA = AP$.

□

That is, when we see $\mathrm{Aut}(X)$ as matrices, it is equivalent to the intersection of the centralizer of A with the permutation group. As every permutation matrix is orthogonal, the following property follows from (7):

Proposition 2.17. *If a and b similar, then they are cospectral.*

2.3 Parallel Vertices

The following condition will also be necessary for PST:

Definition 2.18. *Two vertices $a, b \in V(X)$ are **parallel**, denoted by $a \parallel b$, if the vectors $E_r e_a$ and $E_r e_b$ are parallel for each r. Recall that E_r denotes the spectral projection onto the λ_r-eigenspace.*

This definition is purely algebraic, and we are still determining if some purely combinatorial condition is equivalent to it, like the definition of cospectrality. There is no straightforward relationship between two vertices being symmetrical in some sense and them being parallel. A significant counterexample is provided by complete graphs, where all vertices are similar and yet not parallel when we have more than 2 vertices.

Now we shall see another equivalent condition:

Theorem 2.19. *For $a, b \in V(X)$ the following conditions are equivalent:*

(1) $a \parallel b$;

(2) All poles of the rational function $\phi(X \setminus ab, t)/\phi(X, t)$ are simple.

Proof. By Cauchy-Schwarz, $E_r e_a$ and $E_r e_b$ are parallel iff $\langle E_r e_a, E_r e_b \rangle^2 = \|E_r e_a\|^2 \|E_r e_b\|^2$, which is equivalent to $(E_r)_{a,b}^2 = (E_r)_{a,a}(E_r)_{b,b}$. The poles of $\phi(X \setminus ab)$ are simple iff we have for each r

$$\gamma := \left.\frac{(t-\lambda_r)^2 \phi(X \setminus ab)\phi(X,t)}{\phi(X,t)^2}\right|_{t=\lambda_r} = 0,$$

(here we use that the zero of $\phi(X,t) = \prod(t - \lambda_r)$ are precisely λ_r).

Thus, by using Theorem 2.11 we have

$$\begin{aligned}
(E_r)_{a,b}^2 &= \left.\frac{(t-\lambda_r)^2(\phi(X \setminus a, t)\phi(X \setminus b, t) - \phi(X \setminus ab, t)\phi(X,t))}{\phi(X,t)^2}\right|_{t=\lambda_r} \\
&= \left.\frac{(t-\lambda_r)^2(\phi(X \setminus a, t)\phi(X \setminus b, t)}{\phi(X,t)^2}\right|_{t=\lambda_r} - \gamma \\
&= (E_r)_{a,a}(E_r)_{b,b} - \gamma
\end{aligned}$$

from where we conclude that a and b are parallel iff $\gamma = 0$. □

A simple sufficient condition for two vertices being parallel is that all the eigenvalues of the graph are simple. We can say more

Proposition 2.20. *All the vertices of X are pairwise parallel iff all the eigenvalues are simple.*

Proof. The eigenvalues are simple iff $\operatorname{rk} E_r = 1$ for all r; clearly, all vertices will be parallel in this case. Conversely, if all vertices are parallel, we have $E_r e_j \parallel E_r e_k$ for each j, k, which implies that $\operatorname{rk} E_r = 1$. □

The following definition will be very useful when studying PST, and the next proposition will be used in the main theorem of the next section.

Definition 2.21. *The **eigenvalue support** of a vertex a is the set of eigenvalues λ_r such that their related eigenspace projector satisfies $(E_r)_{a,a} \neq 0$.*

Proposition 2.22. *We have $\operatorname{col} W_a = \operatorname{col} W_b$ iff the a and b are parallel and have the same eigenvalue support.*

Proof. $\operatorname{col} W_a$ is composed by vectors of the form $p(A)e_a$, for some $p \in \mathbb{R}[t]$. As $E_r p(A)v = p(\lambda_r)v$, we have $E_r(\operatorname{col} W_a) = \langle E_r e_a \rangle$. Also, $I = \sum E_r$ allows us to conclude that $\operatorname{col} W_a = \operatorname{col} W_b$ iff $E_r(\operatorname{col} W_a) = E_r(\operatorname{col} W_b)$ for each r. This happens iff $\langle E_r e_a \rangle = \langle E_r e_b \rangle$ for each r, or, equivalently a and b are parallel with same eigenvalue support. □

2.4 Strong cospectrality

The following definition combines parallel vertices and cospectrality:

Definition 2.23. *We say that the vertices $a, b \in V(X)$ are strongly-cospectral if for each d we have $E_r e_a = \pm E_r e_b$.*

Since $(E_r)_{a,a,} = e_a^* E_r e_a = \|E_r e_a\|$ it is easy to see that a, b are strong-cospectral iff they are cospectral and parallel. As was the case of the other sections, we have a theorem of equivalences:

Theorem 2.24. *For $a, b \in V(X)$, the following conditions are equivalent:*

(1) a, b are strongly-cospectral (that is, $\forall r, E_r e_a = \pm E_r e_b$);

(2) a, b are cospectral and parallel;

(3) $\phi(X \setminus a, t) = \phi(X \setminus b, t)$ and the poles of the rational function $\phi(X \setminus ab, t)/\phi(X, t)$ are simple;

(4) $W_a^* W_a = W_b^* W_b$ and $\operatorname{col} W_a = \operatorname{col} W_b$;

(5) The $\mathbb{R}[A]$-module generated by $e_a + e_b$ and $e_a - e_b$ are orthogonal and their direct sum is the $\mathbb{R}[A]$-module generated by e_a;

(6) There is a symmetric matrix Q that is polynomial in A with $Q^2 = I$ and $Qe_a = e_b$;

(7) There is a polynomial $p \in \mathbb{R}[t]$ such that $p^2(A) = I$ and $p(A)e_a = e_b$.

Proof. (1) $\iff$ (2) was already discussed; (3) follows from Theorem 2.19. (4) follows from condition (4) of Theorem 2.14 together with Proposition 2.22 and the fact that cospectral vertices always have the same spectral support. The first part of (5) is already proved in Theorem 2.14. As

$$e_b = \frac{1}{2}((e_a + e_b) - (e_a - e_b)),$$

we have $(e_a + e_b)_{\mathbb{R}[a]} \oplus (e_a - e_b)_{\mathbb{R}[A]} = (e_a)_{\mathbb{R}[A]}$ iff $e_b = p(A)e_a$ which is equivalent to $\operatorname{col} W_a = \operatorname{col} W_b$. It is clear that (6) and (7) are equivalent. At last, it is clear that (7) implies $\operatorname{col} W_a = \operatorname{col} W_b$ and condition (6) of Theorem 2.14. Now, suppose that a and b are strongly cospectral and let $E_r e_a = \sigma_r E_r e_b$, with $\sigma_r = \pm 1$. Let p be the polynomial such that $p(\lambda_r) = \sigma_r$ where λ_r is the eigenvalue related to E_r, and $p(\lambda_r) = 1$ when λ_r is not in the eigenvalue support of a. It is clear that $p^2(\lambda_r) = 1$ for each r, from where $p^2(A) = I$. It is also true that

$$\begin{aligned} p(A)e_a &= p\left(\sum \lambda_r E_r\right) e_a \\ &= \sum p(\lambda_r) E_r e_a \\ &= \sum \sigma_r E_r e_a \\ &= \sum E_r e_b \\ &= e_b, \end{aligned}$$

which concludes the proof.

□

Chapter 3

State transfer

3.1 The unitary group

We will now introduce the main subject of the thesis. For a graph X with adjacency matrix A and Hamiltonian H (as defined in Section 1.1), we define its **unitary group** as:

$$U(t) := e^{itH}.$$

As we can see in [14, 20], this map gives us the solution to Schrödinger's equation and, therefore, provides us with the time evolution of a quantum system. Specifically, at time t, the state of a system originally in the state ψ_0 will be given by $\psi_t = U(t)\psi_0$. Here, these vectors are indexed by the subsets $S \subseteq V(X)$, and the value $|\langle S|\psi_t\rangle|^2$ is the probability of obtaining the qubits in S as 1, and the rest as 0, when the system is measured at time t. We will denote $|\{a\}\rangle =: |a\rangle$, and we observe that the submatrix with singletons as entries is exactly e^{itA}. For more details, see [3, 5, 7].

The map $t \mapsto U(t)$ gives us a group homomorphism with respect to addition in the reals and matrix multiplication [14, 20]. It is worth noting that the eigenvalues of $U(t)$ are of the form $e^{i\lambda t}$ for $t \in \mathbb{R}$ and $\lambda \in \sigma(H)$, making $U(t)$ unitary and justifying the name unitary group.

As $U(t)$ is orthogonal, we can see that if an entry in a $U(t)$ has modulus one at $t = \tau$, the rest of the column must be zero. That is, if $(e^{i\tau A})_{a,b} = \gamma$ with $|\gamma| = 1$, then $U(\tau)|a\rangle = \gamma|b\rangle$, from where:

$$\gamma\langle b|\psi_\tau\rangle = \langle a|U(\tau)^*|U(\tau)|\psi_0\rangle = \langle a|\psi_0\rangle.$$

The above equation means that the probability of measuring the system in the state $|b\rangle$ at time τ is the same as that of obtaining the measure $|a\rangle$ if measured at time 0 instead. This phenomenon is described as that there has been perfect state transfer between vertices a and b.

This discussion leads us to a vital proposition (which we will use as a definition from now on).

Proposition 3.1. *There is perfect state transfer (PST) between vertices a and b at time τ iff $|U(\tau)_{a,b}| = 1$.*

A priori, we should say that the PST occurs *from a to b*. However, as $A^T = A$ we have $(e^{itA})^T = \sum e^{it\lambda_r} E_r^T = e^{itA}$. Hence $(e^{itA})_{a,b} = (e^{itA})_{b,a}$ and there is PST from a to b at time τ iff there is PST from b to a, in which case we say that there is PST *between* these vertices.

3.2 Conditions for perfect state transfer

The results of the rest of the chapter are from [11].

We will now show three inequalities, for which, when equality holds in all of them, it implies the existence of perfect state transfer.

$$\begin{aligned}
|(e^{itA})_{a,b}| &\leq \sum_r |(E_r)_{a,b}| && (3.1)\\
&\leq \sum_r \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}} && (3.2)\\
&\leq \sqrt{\left(\sum_r (E_r)_{a,a}\right)\left(\sum_r (E_r)_{a,a}\right)} && (3.3)\\
&= 1
\end{aligned}$$

Using Proposition 1.5 gives us the first inequality.

Proposition 3.2. *Let X be a graph and E_r be the idempotent of the spectral decomposition of $A(X)$. Then, we have*

$$|(e^{itA})_{a,b}| \leq \sum |(E_r)_{a,b}|,$$

and equality holds iff there is a complex number γ such that

$$e^{t\lambda_r} = \gamma\sigma_r, \qquad \forall r;\ (E_r)_{a,b} \neq 0, \tag{C1}$$

where σ_r is the sign of $(E_r)_{a,b}$

Proof. It follows directly from

$$\begin{aligned}|(e^{itA})_{a,b}| &= |\left\langle e_a, e^{itA} e_b \right\rangle| \\ &= |\sum_r \left\langle e_a, e^{it\lambda_r} E_r e_b \right\rangle| \\ &= |\sum_r e^{it\lambda_r} (E_r)_{a,b}| \\ &\leq \sum_r |(E_r)_{a,b}|.\end{aligned}$$

As we used only the triangle inequality, equality holds iff all $e^{it\lambda_r}(E_r)_{a,b}$ are co-linear and have the same direction , which is equivalent to the condition in the hypothesis. □

The other two conditions for having equality were previously studied. Namely:

$$\sum_r |(E_r)_{a,b}| = \sum_r \sqrt{(E_r)_{a,b}} \sqrt{(E_r)_{b,b}} \iff a \parallel b; \tag{C2}$$

$$\sum_r \sqrt{(E_r)_{a,b}} \sqrt{(E_r)_{b,b}} = 1 \iff a, b \text{ are cospectral.} \tag{C3}$$

The intermediary term has a definition of its own. We note that for any $a \in V(X)$, the numbers $(E_r)_{a,a}$ are non-negative and sum up to one; thus, they define a discrete probability measure, called **spectral density of X with respect to a**. We have proved that a and b have the same spectral density iff they are cospectral.

Definition 3.3. *Given two discrete probability densities, p, q, we define their **fidelity** as*

$$\sum_r \sqrt{p_r q_r}.$$

By Cauchy-Schwarz, the fidelity of two densities is a number in $[0, 1]$ and is 1 iff they are multiples of one another and thus the same. This proves ($C3$), and for ($C2$) we have the following proposition:

Proposition 3.4. *The fidelity of spectral densities of vertices $a, b \in V(X)$ are bounded bellow by $\sum_r |(E_r)_{a,b}|$. Equality holds iff $a \parallel b$.*

Proof. It follows directly from Cauchy-Schwarz:

$$(E_r)_{a,a}(E_r)_{b,b} - ((E_r)_{a,b})^2 = \|E_r e_a\|^2 \|E_r e_b\|^2 - \langle E_r e_a, E_r e_b \rangle^2 \geq 0.$$

Also, equality is obtained in the sum iff $E_r e_a$ is a multiple of $E_r e_b$ for each r, which is the definition of a, b being parallel. □

3.3 Periodicity condition

We say that the vertex a of X is **periodic with period** τ if $U(\tau)e_a = e_a$.

An immediate consequence of having PST between vertices a and b at the time τ is the following:

$$U(2\tau)e_a = U(\tau)(U(\tau)e_a) = U(\tau)e_b = e_a.$$

Thus, we conclude that a necessary condition for having PST involving a vertex a is that e_a is periodic.

Definition 3.5. *We say that* ***the ratio condition*** *on the eigenvalue support of a holds if for any four eigenvalues on the support $\lambda_r, \lambda_s, \lambda_k, \lambda_l$, with $\lambda_k \neq \lambda_l$, we have:*

$$\frac{\lambda_r - \lambda_s}{\lambda_k - \lambda_l} \in \mathbb{Q}.$$

We shall now give a necessary and sufficient condition for a vertex to be periodic.

Proposition 3.6. *A vertex $a \in V(X)$ is periodic iff the ratio condition holds on the eigenvalue support of a.*

Proof. If the vertex a is periodic at time τ, we have

$$\left(\sum_r e^{i\tau\lambda_r} E_r\right) e_a = e_a = \left(\sum_r E_r\right) e_a,$$

multiplying both sides by the conjugate, we have

$$\left(\sum_r e^{i\tau\lambda_r} E_r\right) e_a e_a^* \left(\sum_r e^{-i\tau\lambda_r} E_r\right) = \left(\sum_r E_r\right) e_a e_a^* \left(\sum_r E_r\right),$$

$$\sum_{r,s} e^{i\tau(\lambda_r - \lambda_e)} E_r e_a e_a E_s = \sum_{r,s} E_r e_a e_a^* E_s,$$

and as the matrices $\{E_r e_a e_a^* E_s\}_{r,s}$ are independent we conclude that, for λ_r, λ_s in the eigenvalue support of a,

$$e^{i\tau(\lambda_r - \lambda_s)} = 1.$$

This is equivalent to

$$\tau(\lambda_r - \lambda_s) = m_{r,s} 2\pi, \qquad m_{r,s} \in \mathbb{Z}.$$

Thus, by dividing, we shall get the ratio condition. For the converse, we observe that if the ratio condition holds, we have

$$\frac{\lambda_r - \lambda_s}{\lambda_k - \lambda_l} = m_{r,s,k,t} \in \mathbb{Q}.$$

Taking M as the least common multiple of the divisors of $\{m_{r,s,k,l}\}_{r,s}$, where $\lambda_k \neq \lambda_l$ are fixed, we have:

$$M\frac{\lambda_r - \lambda_s}{\lambda_k - \lambda_l} \in \mathbb{Z}, \qquad \forall r, s;$$

from where, X will be periodic on a with period

$$\tau := \frac{2M\pi}{\lambda_k - \lambda_l}.$$

□

We will present a criterion for the ratio condition to hold on a set of algebraic integers. But we recall some concepts beforehand. We say that two reals a, b are **algebraic conjugates** if there is an irreducible polynomial $p \in \mathbb{Q}[t]$ such that $p(a) = p(b) = 0$. The numbers that are roots of **monic** polynomials with coefficients in $\mathbb{Z}$ are called **algebraic integers**, and form a ring. All algebraic integers are either integers or irrational. A real irrational number μ is said to be a quadratic integer if it is the root of a second-degree monic polynomial in $\mathbb{Z}$. This is equivalent [11] to having one of the following conditions for a square-free $\Delta > 1$:

- $\mu = a + b\sqrt{\Delta}$ and $\Delta \equiv 2, 3 \mod 4$;
- $\mu = \frac{1}{2}(a + b\sqrt{\Delta})$ with $\Delta \equiv 1 \mod 4$ and $a \equiv b \mod 2$.

The eigenvalues of a symmetric matrix with integer coefficients are the roots of a monic integer polynomial. Thus, we can use the following theorem:

Theorem 3.7. *Let $S = \{\lambda_0, \ldots, \lambda_d\}$ be a set of real algebraic integers, closed under taking algebraic conjugates, with $d \geq 3$. Then, the ratio condition holds for S iff either holds*

- *The elements of S are integers.*
- *The elements in S are quadratic integers, and there is a square-free $\Delta > 1$, and integers $a, b_0, \ldots, b_d$ such that $\lambda_r = \frac{1}{2}(a + b_r\sqrt{\Delta})$.*

Proof. A simple calculation shows us that we have the ratio condition if either holds. For the converse, we observe that if two elements, λ_0 and λ_1, are integers, then

$$\frac{\lambda_r - \lambda_0}{\lambda_0 - \lambda_1} \in \mathbb{Q},$$

and since the algebraic integers are either irrational or integers, we conclude that λ_r is an integer. Thus, the first case holds.

Now, if there is at most one integer, we will show that $(\lambda_0 - \lambda_1)^2 \in \mathbb{Z}$. By the ratio condition, for each pair r, s we have $a_{r,s} \in \mathbb{Q}$ such that

$$\lambda_r - \lambda_s = a_{r,s}(\lambda_0 - \lambda_1),$$

from where

$$\prod_{r\neq s}(\lambda_r - \lambda_s) = (\lambda_0 - \lambda_1)^{d^2-d}\prod_{r\neq s} a_{r,s}.$$

Since the left side is fixed by any field automorphism of $\mathbb{Q}[\lambda_0, \dots, \lambda_d]$, it must be an integer; and as the product of the $a_{r,s}$ is rational, we have

$$(\lambda_0 - \lambda_1)^{d^2-d} \in \mathbb{Q}.$$

As $\lambda_0 - \lambda_1$ is algebraic integer, we have

$$(\lambda_0 - \lambda_1)^{d^2-d} \in \mathbb{Z}.$$

This means that $(\lambda_0 - \lambda_1)$ is an integer multiple of a root of unity, and since the set is closed under taking algebraic conjugates and has only real elements, we must have that $(\lambda_0 - \lambda_1)$ is a quadratic integer or integer. In both cases, it is an integer multiple of $\sqrt{\Delta}$, for a square-free positive integer Δ. Since

$$(\lambda_r - \lambda_0)^2 = a_{r,0}^2(\lambda_0 - \lambda_1)^2,$$

it follows that $(\lambda_r - \lambda_0)^2$ is rational and thus $\lambda_r - \lambda_0$ is integer multiple of $\sqrt{\Delta_r}$, where Δ_r is a square-free natural. Since the square-free part of $(\lambda_r - \lambda_0)^2$ is the same as $(\lambda_0 - \lambda_1)^2$ we have $\Delta_r = \Delta$. Therefore, we have integers m_r such that:

$$\lambda_r = \lambda_0 - m_r\sqrt{\Delta}.$$

When we sum all elements on S, we obtain

$$|S|\lambda_0 - \sqrt{\Delta}\sum m_r = \sum \lambda_r,$$

which is an integer since the sum of all roots of a polynomial corresponds to the opposite of its term of the second largest degree. Therefore, we have $\lambda_0 \in \mathbb{Q}(\sqrt{\Delta})$ as well as the other elements. Their rational parts are the same, for their difference is an entire multiple of $\sqrt{\Delta}$. □

Corollary 3.8. *Let X be an integer-weighted graph and S be the eigenvalue support of the vertex a. Then X is periodic at a iff one of the following holds*

- *The elements of S are integers.*
- *The elements in S are quadratic integers, and there is a square-free $\Delta > 1$, and integers $a, b_0, \dots, b_d$ such that $\lambda_r = \frac{1}{2}(a + b_r\sqrt{\Delta})$.*

Moreover, if $e^{itA}e_a$ is not constant, and taking $\Delta = 1$ if the eigenvalues are integers, we conclude that the smallest period is

$$\tau = \frac{2\pi}{g\sqrt{\Delta}},$$

where

$$g := \gcd\left\{\frac{\lambda - \lambda_r}{\sqrt{\Delta}}\right\}_{\lambda_r \in S},$$

for some arbitrary $\lambda \in S$.

Proof. If $|S| = 1$, then $e^{itA}e_a$ is constant up to a phase. S will be closed under algebraic conjugation, since if λ_r and λ_s are conjugated then so are E_r and E_s and $E_r e_a = 0$ iff $E_s e_a = 0$. If $|S| = 2$, its elements are integers or quadratic integers, satisfying one of the conditions. For $|S| \geq 3$, we use Proposition 3.6 and Theorem 3.7. If periodicity holds at τ, we can write

$$\tau = x\frac{2\pi}{g\sqrt{\Delta}},$$

where $x \in \mathbb{R}$. From the proof of Proposition 3.6, we see that

$$x\frac{\lambda - \lambda_r}{g\sqrt{\Delta}} \in \mathbb{Z},$$

so with this choice of g, it follows that x is an integer, and also, this is the greatest value that does so. Hence this period is minimal. □

We observe that as b_n are integers, we must have that

Corollary 3.9. *If $a \in V(X)$ is periodic, then the elements of the eigenvalue support of a have a distance of at least 1 from each other.*

A stronger result holds: if We have PST between a and b, then the values in its support have distance at least $\sqrt{2}$. [13]

3.4 The equivalence theorem

We start with a definition of a norm on $\mathbb{Q}$. Given $t \in \mathbb{Q}$, we can write $t = p^{\alpha}(r/s)$ with r, s integers without the factor p. Then, we define the p-adic norm of t as

$$\|t\|_p := p^{-\alpha}.$$

If we denote by λ_0 the largest eigenvalue (which is also the norm of the matrix) of a graph X, then by Perron-Frobenius, it must be in the eigenvalue support of each vertex. The main theorem of perfect state transfer is

Theorem 3.10. *Let a, b be vertices of a connected graph X and let $S = \{\lambda_0, \ldots, \lambda_k\}$ be the eigenvalue support of a. There is PST between a and b iff the three conditions are satisfied:*

(1) a and b are strongly cospectral;

(2) The eigenvalues of S are either integers or quadratic integers; and moreover there are integers $\Delta, p, q_0, \ldots, q_k$ with $\Delta > 0$ and square-free such that

$$\lambda_r = \frac{1}{2}(p + q_r\sqrt{\Delta});$$

(3) Let us denote by λ_0 the spectral radius. There is a non-negative α such that

- $(E_r)_{a,b} > 0$ *iff* $\|(\lambda_0 - \lambda_r)/\sqrt{\Delta}\|_2 < 2^{-\alpha}$;
- $(E_r)_{a,b} < 0$ *iff* $\|(\lambda_0 - \lambda_r)/\sqrt{\Delta}\|_2 = 2^{-\alpha}$.

If the above conditions hold, the minimum period for PST between a and b is

$$\tau = \frac{\pi}{g\sqrt{\Delta}},$$

where

$$g := \gcd\left\{\frac{\lambda_0 - \lambda_r}{\sqrt{\Delta}}\right\}_{r=1,\ldots,k}.$$

Proof. We already know that conditions (1) and (2) are necessary. Thus, we suppose that they are satisfied and show that (3) is equivalent to having PST. (1) implies that the eigenvalue support of a and b are the same, and (2) implies that if PST occurs, it must be on half of the period, that is, for the chosen value for τ. We have

$$e^{i\tau A}e_a = \gamma e_b \iff \forall\lambda_r,\ e^{i\tau\lambda_r}E_r e_a = \gamma E_r e_b.$$

As E_0 has positive entries, this condition is equivalent to have $\gamma = e^{i\tau\lambda_0}$ and

$$e^{i\tau(\lambda_0-\lambda_r)} = \pm 1,$$

where the sign is the sign of $(E_r)_{a,b}$. This expression is equivalent to having $(\lambda_0-\lambda_r)/g\sqrt{\Delta}$ even if $(E_r)_{a,b} > 0$ and odd otherwise, which is equivalent to the condition stated in (3) □

Corollary 3.11. *If there is PST between a and b, and between b and c, we must have $a = c$.*

Proof. The time when we have PST does not depend on the vertex, only on its eigenvalue support, which must be the same for a, b, c since they are (strongly-)cospectral. □

Chapter 4

Some graphs and PST

We have chosen to present some examples after discussing the basic properties so that we can better analyze what is being illustrated in them. Let us begin with the simplest case, the graph P_2, which exhibits perfect state transfer between vertices. The existence of PST can be deduced through a straightforward calculation using the adjacency matrix.

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad e^{itA} = \sum_n \frac{(it)^n}{n!} A^n.$$

Here, we can use that $A^2 = I$ to calculate the sum as

$$\sum_n \frac{(it)^n}{n!} A^n = \sum_{2|n} \frac{(it)^n}{n!} I + \sum_{2\nmid n} \frac{(it)^n}{n!} A = \begin{pmatrix} \cos t & i\sin t \\ i\sin t & \cos t \end{pmatrix},$$

hence there is perfect state transfer at time $t = \pm\frac{\pi}{2}$.

In general, we can repeat this argument to compute the unity group of a bipartite graph. If we choose an appropriate order on the vertices, the adjacency matrix will be of the form

$$A = \begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix},$$

from where a similar computation will give us:

$$e^{itA} = \begin{pmatrix} \cos(t\sqrt{BB^*}) & i\sin(t\sqrt{BB^*})B \\ i\sin(\sqrt{BB^*})B^* & \cos(\sqrt{tB^*B}) \end{pmatrix}.$$

Analyzing under Theorem 3.10, the eigenvalues of P_2 are ± 1, hence simple. From this and using that the vertices are similar, they must be strongly cospectral. Finally, the last condition is satisfied since calling $\lambda_0 = 1$ and $\lambda_1 = -1$ we have $E_1 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$, $\|\lambda_0 - \lambda_1\|_2 = \frac{1}{2}$ and $(E_1)_{0,1} < 0$.

A similar analysis allows us to conclude that P_3 has PST between the extremities.

4.1 Some non-examples

4.1.1 Complete graph

At first, it would seem like we would have PST between any two vertices of K_n due to their extreme symmetry. However, this cannot happen due to Corollary 3.11. Well, no two vertices of K_n are even parallel.

The spectral decomposition of $A(K_n)$ is

$$A = J - I = (n-1)\left(\frac{1}{n}J\right) - 1\left(I - \frac{1}{n}J\right).$$

where $(1/n)J$ is the projector onto $\mathbb{1}$, which is the Perron eigenvector of the graph, and $I - (1/n)J$ is the projector onto $\mathbb{1}^\perp$. We could do a direct calculation to show that there are no two strongly cospectral vertices if $n > 2$; instead, we shall use an already seen proposition together with:

Proposition 4.1. *Graph isomorphism preserves cospectrality, parallelism, and PST.*

Proof. Let X, Y be graphs and $\varphi\colon X \to Y$ an isomorphism. Denoting by A and B their adjacency matrices, respectively, and P the permutation related to φ, we have $B = PAP^*$. The spectra of A and B are the same; and if ξ is A-eigenvector related to λ_r, then $P\xi$ must be a B-eigenvector related to λ_r, for

$$BP\xi = PAP^*P\xi = P(A\xi) = \lambda_r P\xi.$$

Thus, denoting by E_r, F_r the spectral projectors of X, Y, respectively, we have:

$$F_r = \sum (P\xi)(P\xi)^* = P\left(\sum \xi\xi^*\right)P^* = PE_rP^*,$$

where the sum is over the eigenvectors related to λ_r.

From that, we conclude that

$$E_r e_a = \pm E_r e_b \iff PE_rP^*Pe_a = \pm PE_rP^*Pe_b \iff F_r e_{\varphi(a)} = F_r e_{\varphi(b)}.$$

Since P preserves angles, we have

$$\begin{aligned} E_r e_a \parallel E_r e_b &\iff PE_r e_a \parallel PE_r e_b \\ &\iff PE_rP^*Pe_a \parallel PE_rP^*Pe_b \\ &\iff F_r e_{\varphi(a)} \parallel F_r e_{\varphi(b)}; \end{aligned}$$

Also,

$$\begin{aligned}\|e_a^* e^{itA} e_b\| = 1 &\iff \|e_a^* P P^* e^{itA} P^* P e_b\| = 1 \\ &\iff \|e_{\varphi(a)}^* e^{itB} e_{\varphi(b)}\| = 1.\end{aligned}$$

which concludes the proof. □

We can use this proposition to show that there are now two parallel vertices in K_n ($n > 2$). If a, b are parallel in K_n, then each vertex must be parallel to each other, and thus we would have to have simple spectrum by Proposition 2.20, which is absurd since K_n ($n > 2$) does not have a simple spectrum. In particular, this shows us that Proposition 2.17 does not generalize for parallelism.

Proposition 4.2. *There is no pair of parallel vertices in K_n for $n > 2$. In particular, we do not have strong-cospectrality or PST.*

4.1.2 Paths

Another important class of graphs that we shall discuss is the path graphs. Is there PST in P_d?

The answer will be negative for $d > 3$, as we will see ahead, but beforehand we will see some properties of the graph. The adjacency matrix will be

$$P_d = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}.$$

Denoting by

$$C := \begin{pmatrix} 0 & 1 & & & \\ 0 & 0 & 1 & & \\ & 0 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 0 & 0 \end{pmatrix},$$

we have $P = C + C^*$. The effect of C on a vector is to shift its entries to the left (and put a zero at the end), hence if we call $\xi := \begin{pmatrix} \omega & \omega^2 & \cdots & \omega^d \end{pmatrix}$, where $\omega^{d+1} = -1$, we shall have that $C\xi = \omega\xi + e_d$. Using that C^* is the right-shift and that $\overline{\omega} = \omega^{-1}$ we can conclude that

$$\begin{aligned} C^*\xi &= \overline{\omega}\xi + e_1, \\ C(-\overline{\xi}) &= -(\overline{C\xi}) = -\overline{\omega}\overline{\xi} - e_d, \\ C^*(-\overline{\xi}) &= -\omega\overline{\xi} - e_1, \end{aligned}$$

from where

$$(C + C^*)(\xi - \overline{\xi}) = (\omega + \overline{\omega})(\xi - \overline{\xi}).$$

Thus, the eigenvalues of P_d are of the form $\omega + \overline{\omega}$, if $\omega^{d+1} = -1$, that is:

$$2\Re(\omega) = 2\cos\left(\frac{\pi k}{d+1}\right), \qquad k = 1, \ldots, d.$$

In particular, as they are distinct, P_d must have a simple spectrum, and all the vertices must be parallel.

The matrix

$$R = \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & \iddots & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix}$$

is an automorphism on P_d, from where all the opposite vertices on the path are isomorphic, thus cospectral and strongly cospectral.

The following proposition implies the nonexistence of PST in a class of paths. For this, we make use of the lower bound of the Euler's totient function

$$\phi(n) \geq \frac{\sqrt{n}}{\sqrt{2}},$$

whose proof can be found on [22].

Proposition 4.3. *For $d \geq 6$, no vertex of P_d is periodic.*

Proof. As $\sigma(P_d) \subseteq (-2, 2)$, it suffices to show that the eigenvalue support of each vertex has cardinality at least 5 and use Corollary 3.9. Each spectral projector is of the form

$$E_r = (\xi - \overline{\xi})(\xi - \overline{\xi})^*,$$

from where

$$(E_r)_{a,a} = (2\Im(\omega^a))^2,$$

which is non-zero for every ω primitive $(2d+2)$-th root of unit. We have $\phi(2d+2)$ primitive $(2d+2)$-th roots. Using the above bound, we have $\phi(n) \geq 5$ for $n \geq 50$. Moreover, we can verify that $\phi(n) \geq 5$ for $13 \leq n \leq 50$. This implies that for $d \geq 6$, there is no periodic vertex on P_d. □

There is no PST in P_d for $d \geq 4$. We can check individually the remaining cases or use a more general argument, specific for PST, as in [11].

4.2 How to construct new graphs

In this work, we shall see two ways of building new graphs, starting from other ones that ensure some properties are kept. We have two main techniques: one will be using Cartesian maps, which will be seen now, and the other is by using equitable partitions, which will be postponed to Section 6.4.

The main tool in this section is the following

Definition 4.4. *Let X, Y be graphs. We define the* ***Cartesian product*** *graph $X \square Y$ as the graph in $V(X) \times V(Y)$ where*

$$(a, b) \sim (a', b') \iff \begin{cases} a = a', b \sim b' \\ a \sim a', b = b' \end{cases} .$$

Or, equivalently, as the graph whose adjacency matrix is given by

$$A(X \square B) = A(X) \oplus A(Y).$$

We denote by $X^{\square n}$ the Cartesian product of X with itself n times.

Now we have the main theorem of the section.

Theorem 4.5. *A necessary and sufficient condition for there to exist PST between (a, b) and (a', b') in the graph $X \square Y$ with minimal time τ is that there exists PST between a and a' in X with minimal period τ_1, and PST between b and b' in Y with minimal period τ_2, such that $\tau_1/\tau_2 = p/q$ with p and q odd and coprime integers. In that case, $\tau = \tau_1 q = \tau_2 p$.*

Proof. ($\Rightarrow$) If there is PST in $X \square Y$ at τ we have, using Proposition 1.3:

$$e^{i\tau X} e_a \otimes e^{i\tau Y} e_b = e^{i\tau(X \oplus Y)}(e_a \otimes e_b) = e_{a'} \otimes e_{b'},$$

from where

$$e^{i\tau X} e_a = e_{a'}, \quad e^{i\tau Y} e_b = e_{b'}.$$

Now let us show that the minimum periods of the PST of a, a' and b, b' satisfy the conditions. Denote by τ_1 the minimal time on X and τ_2 on Y. As τ is a period for PST in a, a' and b, b' there must be odd positive integers k_1, k_2 for which

$$\tau_1 k_1 = \tau = \tau_2 k_2$$

from where we get that $\tau_1/\tau_2 = k_2/k_1$. The converse is immediate using Proposition 1.3. $\square$

Corollary 4.6. *A necessary and sufficient condition for there to exist PST between (a,b) and (a,b') in the graph $X\square Y$ with minimal time τ is that a is periodic with minimal period τ_1; and there is PST between b and b' in Y with minimal period τ_2, such that $\tau_1/\tau_2 = p/q$ with p and q coprime and p odd. In that case, $\tau = \tau_1 q = \tau_2 p$.*

Corollary 4.7. *If there is PST between a,b at minimal time τ in X, then there is PST between $(a,a,\ldots,a),(b,b,\ldots,b)$ in $X^{\square n}$ at minimal time τ.*

Another important information that we need to study the product of graphs is the distance between vertices, which is easily computed by the following proposition.

Proposition 4.8. *For $a,a' \in X$ and $b,b' \in Y$ we have*

$$d_{X\square Y}((a,b),(a',b')) = d_X(a,a') + d_Y(b,b').$$

Proof. It is clear that there is a path from (a,b) to (a',b) of length $d_X(a,a')$, and similarly for (a',b) to (a',b'), which gives us

$$d_{X\square Y}((a,b),(a',b')) \leq d_X(a,a') + d_Y(b,b').$$

For the converse, let $d = d_{X\square Y}((a,b),(a',b'))$, and let A and B be the adjacency matrices of X and Y, respectively. Then, we have:

$$\begin{aligned} 0 < (A \oplus B)^d_{(a,b),(a',b')} &= (A\otimes I + I \otimes B)^d_{(a,b),(a',b')} \\ &= \left(\sum \binom{d}{r} (A^r \otimes B^{d-r})\right)_{(a,b),(a',b')} \\ &= \sum \binom{d}{r} (A^r_{a,a'} \cdot B^{d-r}_{b,b'}), \end{aligned}$$

which implies that $A^r_{a,a'} > 0$ and $B^{d-r}_{b,b'} > 0$ for some $r \leq d$. Therefore, we have

$$d_X(a,a') \leq r \quad \text{and} \quad d_Y(b,b') \leq d-r \implies d_X(a,a') + d_Y(b,b') \leq d.$$

$\square$

We note that a simple combinatorial argument shows that $|E(X\square Y)| = |E(X)||V(Y)| + |V(X)||E(Y)|$ and $|V(X\square Y)| = |V(X)||V(Y)|$. Combining all the arguments, we see that in the d-cube $P_2^{\square d}$, the distance between two extreme vertices is d, and they have PST. However, the number of edges in the n-cube is $2^{n-1}n$, which means that the number of edges increases exponentially with respect to the distance of the vertices involved in PST. The Cartesian products of paths give us an example of an infinite class of graphs with

PST between vertices of any distance, but the number of edges explodes as the distance increases.

In general, if a graph X has PST between vertices of distance d, then taking the Cartesian product $X^{\square n}$ yields graphs that have PST between vertices with distance dn. However, the number of edges in $X^{\square n}$ is exponential in n, specifically $E(X)^n = O(E(X^{\square n}))$. This topic will be revisited in the final chapter.

Another property that the Cartesian product preserves is cospectrality. We have the main theorem:

Theorem 4.9. *Suppose $a_1, \ldots, a_n$ are cospectral vertices in X and $b_1, \ldots, b_m$ are cospectral vertices in Y. Then the vertices (a_r, b_s) are cospectral in $X \square Y$, for any $1 \leq r \leq n$ and $1 \leq s \leq m$. The same is valid by replacing the term cospectral with similar.*

Proof. Let $A = \sum \lambda_r E_r$, and $B = \sum \mu_s F_s$ be the spectral decomposition of the adjacency matrices of X and Y, respectively. By hypothesis $(E_r)_{a_j,a_j}$ is constant in j, as well as $(F_s)_{b_j,b_j}$, thus $(E_r \otimes F_s)_{(a_j,b_k),(a_j,b_k)}$ is constant in j, k. We can write $A \oplus B$ as

$$A \oplus B = \sum_{r,s} (\lambda_r + \mu_s) E_r \otimes F_s,$$

where $E_r \otimes F_s$ are orthogonal projectors.

This may not be the spectral decomposition once we can have $\lambda_r + \mu_s = \lambda_{r'} + \mu_{s'}$. However, the spectral projectors will be the sum of some $E_r \otimes F_s$, and their sum will also be constant in the wanted entries.

The other part follows directly from the fact that if P and Q commute with A and B, respectively, then $P \otimes Q$, $I \otimes Q$ and $P \otimes I$ commute with $A \oplus B$, together with Proposition 2.16. $\square$

This theorem tells us that the Cartesian product of graphs preserves some combinatorial properties of the original graphs. We observe that $\sigma(X \square Y) = \sigma(X) + \sigma(Y)$, and if we can ensure that $\sigma(X) + \sigma(Y)$ is simple, we can force $X \square Y$ to have several strongly cospectral vertices.

4.3 Distance between vertices with PST and the size of the graph

The main problem that motivated this thesis is the following:

Problem 4.1. *How to construct a simple graph X which possesses PST between two vertices with distance d with the least number of edges.*

We will denote

$$\mathfrak{D}(d) := \min\{|V(X)|\colon X \text{ has two vertices at distance at least } d \text{ with PST}\}.$$

We observe that as $|E(X)|$ is bounded by a polynomial on $|V(X)|$, they must have similar asymptotic behavior. We chose to use $|V(X)|$ in this definition since it is usually easier to compute. The following result is due to Coutinho, [8]:

Theorem 4.10. *We have the bound*

$$\mathfrak{D}(n) > (n/3)^{3/2}.$$

For this proof, we will need the following definition and lemma. The eccentricity of a vertex a in a graph X is the maximum distance between a and another vertex. It is denoted by ϵ_a. Then we have

Lemma 4.11. *Let X be a graph with adjacency matrix A, and $a \in V(X)$. Denote by Φ_a the eigenvalue support of a. Then*

$$\varepsilon_a + 1 \leq |\Phi_a|.$$

Proof. We can consider the subspace of $\mathbb{R}^n$ defined by:

$$W_a = (\{A^r e_a\}_r) = (\{E_r e_a\}_{r \in \Phi_a}),$$

which has dimension $|\Phi_a|$. The support of $A^r e_a$ contains the vertices at a distance r from a and does not contain the vertices at a distance greater than r. Hence, the vectors $\{A^r e_a\}_0^{\varepsilon_a}$ are independent, from where the lemma follows. □

Lemma 4.12. *Let X be a graph with $|E(X)| = m$ with $a \in V(X)$ periodic. Then*

$$\left(\frac{\varepsilon_a}{3}\right)^3 < 2m.$$

Proof. Let τ be the period of a, and let $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ be the eigenvalues of X ordered in non-increasing absolute value. Since the diagonal of A^2 contains the degree of each vertex, we have:

$$\operatorname{tr} A^2 = 2m = \sum_{r=0}^{n-1} \lambda_r^2.$$

From this, it follows that:

$$\lambda_r^2 \leq \frac{2m}{r+1}.$$

Let $k = \lfloor \sqrt[3]{2m} \rfloor$. We can observe that $k \leq n-1$. According to Corollary 3.9, the distance between any two distinct eigenvalues in Φ_a is at least 1. Since:

$$\Phi_a \setminus \{\lambda_0, \ldots, \lambda_k\} \subseteq [-|\lambda_k|, |\lambda_k|],$$

we can conclude that even in the worst-case scenario where $\lambda_0, \lambda_1, \ldots, \lambda_{k-1} \in \Phi_a$, we still have:

$$(|\Phi_a| - k - 1) \leq 2|\lambda_k|,$$

which implies:

$$|\Phi_a| \leq 2\sqrt{\frac{2m}{k+1}} + k + 1 < 2\sqrt[3]{2m} + \sqrt[3]{2m} + 1.$$

This inequality, along with the previous lemma, completes the proof. ☐

Proof of Theorem 4.10. Now, the proof of the main theorem follows trivially from the lemmas and the fact that $|E(X)| \leq \binom{|V(X)|}{2} < \frac{|V(X)|^2}{2}$. ☐

As far as our current knowledge extends, the lower bound presented for $\mathfrak{D}(n)$ is the best known. The example of $P_2^{\square n}$ demonstrates that $\mathfrak{D}(2n) \leq 2^n$. Moreover, utilizing the results from Corollary 4.7 and Proposition 4.8, we can infer that $\mathfrak{D}(kn) \leq \mathfrak{D}(n)^k$. Therefore, we have:

$$\mathfrak{N} := \lim \frac{\log_2(\mathfrak{D}(n))}{n} = \inf \frac{\log_2(\mathfrak{D}(n))}{n}.$$

Proof. Let $a_n := \log_2(\mathfrak{D}(n))$ and $L = \inf(a_n/n)$. Fix $\epsilon > 0$. There exists N such that $a_N/N < L + \epsilon$. Also, there is a value of J for which if $k > J$, then $\frac{k+1}{k} < 1 + \epsilon$. For $m > JN$, we can write $m = kN + r$ with $r < N$ and $k > J$. Consequently, we have $a_m \leq a_{(k+1)N} \leq (k+1)a_N$, and since $m > kN$, we get:

$$\frac{a_m}{m} \leq \frac{(k+1)a_N}{kN} \leq \left(\frac{k+1}{k}\right)\frac{a_N}{N} \leq (1+\epsilon)(L+\epsilon) = L + \epsilon(1 + L + \epsilon).$$

Since $\epsilon > 0$ is arbitrary, we can conclude that a_n/n tends to L, as desired.

☐

The number $\mathfrak{N}$ quantifies the exponential growth of $\mathfrak{D}$. Specifically, for $\alpha > 0$, we have $\mathfrak{D}(n) = O(\alpha^n)$ iff $\mathfrak{N} \leq \log_2 \alpha$. Furthermore, $\mathfrak{D}(n)$ exhibits sub-exponential growth iff $\mathfrak{N} = 0$.

The graph P_2 give us that $\mathfrak{N} \leq 1$ and P_3 implies $\mathfrak{N} \leq \frac{1}{2}\log_3(2) \approx 0.792$.

In Section 6, we will provide bounds for $\mathfrak{N}$ to analyze its properties further.

Chapter 5

Paths with weights

The smallest graph with vertices at a distance d is the path graph P_d. Ideally, we would like to obtain PST using this graph. However, as seen in Subsection 4.1.2, path graphs do not have PST, except for P_2 and P_3. To address this issue, we can add weights to the edges of the path and then create a related simple graph that exhibits properties similar to the weighted paths. This Chapter will explore how to construct weighted paths with PST or other spectral properties. In Chapter 6, we will focus on solving the latter problem.

A preliminary observation is that the concepts in which we are working naturally extend to weighted graphs through the use of the adjacency matrix, which now contains numbers in $\mathbb{R}$ instead of 0 or 1. Two vertices are considered cospectral if any of the conditions outlined in 2.14 are met. Similarly, vertices are labeled as strongly cospectral if they fulfill any of the conditions mentioned in 2.24. Additionally, the Hamiltonian and PST can be defined using identical formulas on $A(X)$.

Consequently, the validity of Theorem 3.10 remains intact even when applied to weighted graphs, as its proof relies solely on linear algebra principles.

5.1 Orthogonal polynomials

In this section, we present a concise introduction to the topic of orthogonal polynomials. We based mainly on [4], where there is a much deeper presentation of the theme.

We have many ways to define a bilinear application in $\mathbb{R}[t]$, considering it as an $\mathbb{R}$-vector space. Let $\langle \cdot, \cdot \rangle_{\mathcal{P}}$ be such a map. It is clear that $\{t^n\}$ forms a basis for the space and that for any $p = \sum a_r t^r$ and $q = \sum b_r t^r$ we have

$$\begin{aligned}\langle p, q\rangle_{\mathcal{P}} &= \left\langle \sum a_r t^r, \sum b_s t^s \right\rangle_{\mathcal{P}} \\ &= \sum_{r,s} a_r b_s \langle t^r, t^s\rangle_{\mathcal{P}} \\ &=: \sum_{r,s} a_r M_{r,s} b_s;\end{aligned}$$

thus, considering the isomorphism inclusion $\mathbb{R}[t] \hookrightarrow \mathbb{R}^{\mathbb{N}}$, given by $t^k \hookrightarrow e_k$, we have $\langle p, q\rangle_{\mathcal{P}} = p^* M q$. We observe that the polynomials correspond to vectors with bounded support; hence, the sum is always finite and well-defined despite the matrix M possibly having infinite non-zero entries.

We are particularly interested in the case in which the operator multiplication by t, defined by $p \mapsto tp$, is self-adjoint considering $\langle \cdot, \cdot\rangle_{\mathcal{P}}$, which happens iff

$$\langle t^r, t^s\rangle_{\mathcal{P}} = \left\langle 1, t^{r+s}\right\rangle_{\mathcal{P}} \quad \forall r, s,$$

and hence, by calling $m_r := \langle 1, t^r\rangle_{\mathcal{P}}$, the matrix associated with the bilinear application will be

$$M_{r,s} = m_{r+s},$$

$$M = \begin{pmatrix} m_0 & m_1 & m_2 & \cdots \\ m_1 & m_2 & m_3 & \cdots \\ m_2 & m_3 & m_4 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

In particular, M is self-adjoint, so the bilinear application is symmetric. We can characterize the semidefinite bilinear applications by:

Theorem 5.1. *Let $\langle \cdot, \cdot\rangle_{\mathcal{P}}$ be a bilinear application on $\mathbb{R}[t]$. The following statements are equivalent:*

(1) The bilinear application is positive semidefinite, and the multiplication by t is self-adjoint;

(2) The matrix related to the bilinear application is of the form

$$M = \begin{pmatrix} m_0 & m_1 & m_2 & \cdots \\ m_1 & m_2 & m_3 & \cdots \\ m_2 & m_3 & m_4 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix};$$

and is positive and semidefinite;

(3) The bilinear application is of the form

$$\langle f, g\rangle_{\mathcal{P}} = \int fg \,\mathrm{d}\mu;$$

for some Borel measure μ.

The equivalence between (1) and (2) comes from the above discussion, and the equivalence between (2) and (3) is known as the Hamburger moment problem and can be found in [4].

Using this theorem, we have

$$\langle f, f\rangle_{\mathcal{P}} = 0 \iff f = 0 \quad \mu\text{-a.e.}.$$

Recall that we say that $f = 0$ μ-almost everywhere, or μ-a.e., if $\mu(f^{-1}(\{0\}^c)) = 0$. Moreover, we define the support of a measure as the set of points whose every neighborhood has a positive measure.

When the support of μ is infinite, $f = 0$ μ-a.e. implies that f has an infinite number of roots, which happens only when $f = 0$, and hence $\langle\cdot,\cdot\rangle_{\mathcal{P}}$ is an inner product.

The other case, which is the one to be analyzed, is when the Borel measure μ has finite support. In this case, the measure is of the form

$$\mu = \sum_{r=0}^{d} \alpha_r \delta_{\lambda_r}, \qquad \alpha_r > 0;$$

for some $d \in \mathbb{N}$, $\lambda_r \in \mathbb{R}$; where δ_{λ_r} is the Dirac measure at λ_r, defined by

$$\delta_{\lambda_r}(B) = \begin{cases} 1 & 1 \in B \\ 0 & 1 \notin B \end{cases}.$$

In this case, the bilinear form will be given by:

$$\langle f, g\rangle_{\mathcal{P}} = \sum \alpha_r f(\lambda_r) g(\lambda_r).$$

A polynomial p will have a null quadratic form iff λ_r is a root for each r. Hence, $\langle p, p\rangle_{\mathcal{P}} = 0$ is equivalent to $\phi := \prod(t - \lambda_r) \mid p$, and from that, we conclude that the kernel of the quadratic application is the ideal $(\phi)_{\mathbb{R}[t]}$.

In other words, the application $\langle\cdot,\cdot\rangle_{\mathcal{P}}$ is constant in the co-sets of $\mathbb{R}[t]/(\phi)$, and this allows us to project the function to the quotient

$$\langle\cdot,\cdot\rangle_{\sigma} : \mathbb{R}[t]/(\phi) \times \mathbb{R}[t]/(\phi) \to \mathbb{R},$$

$$\langle f + (\phi), g + (\phi)\rangle_{\sigma} = \langle f, g\rangle_{\mathcal{P}}.$$

The bilinear map $\langle\cdot,\cdot\rangle_{\sigma}$ is an inner product on $\mathbb{R}[t]/(\phi) \cong \mathbb{R}^{d+1}$ where the index r of λ_r goes from 0 to d. We remember that for a polynomial $p = \sum a_r t^r$ of degree d, the property $p(\lambda_r) = y_r$ can be expressed as the following matrix equation involving the Vandermond matrix of $\{\lambda_r\}_r$, given by $V_{m,n} = \lambda_{m-1}^{n-1}$:

$$\begin{pmatrix} 1 & \lambda_0 & \lambda_0^2 & \dots & \lambda_0^d \\ 1 & \lambda_1 & \lambda_1^2 & \dots & \lambda_1^d \\ 1 & \lambda_2 & \lambda_2^2 & \dots & \lambda_2^d \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_d & \lambda_d^2 & \dots & \lambda_d^d \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_d \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_d \end{pmatrix}.$$

That is, the matrix associated to the inner product will be of the form

$$\langle p, q \rangle_\sigma = p^* V^* \Delta V q,$$

where Δ is the diagonal matrix with α_r.

We observe that as $\deg(\phi) = d + 1$, the polynomials $\{1, t, t^2, \dots t^d\}$ form a basis, and thus we can use Hilbert-Schmidt to produce a basis of orthogonal polynomials, $\{P_0, P_1, \dots, P_d\}$ with $\deg(P_r) = r$. This process determines the basis uniquely up to multiplication by a scalar.

5.2 From orthogonal polynomials to tridiagonal matrices

Let V be the quotient of the spaces of polynomials by a bilinear form that is induced by a finite-supported measure. Call $\langle \cdot, \cdot \rangle_\sigma$ the inner product induced on the quotient. Suppose that we have an orthogonal basis $\{P_0, P_1, \dots, P_d\}$ with $\deg(P_r) = r$. In particular, each P_r is orthogonal to every polynomial q with $\deg(q) < r$ and using that $\langle tP_r, q \rangle_\sigma = \langle P_r, tq \rangle_\sigma$ we have tP_r orthogonal to every polynomial q with $\deg(q) < r - 1$. Writing tP_r on this basis gives us

$$tP_r = \sum_s \frac{\langle tP_r, P_s \rangle_\sigma}{\langle P_s, P_s \rangle_\sigma} P_s,$$

but using the first observation, we have:

Proposition 5.2. *We have sequences* $\{a_r\}_{r=0}^d$; $\{b_r\}_{r=0}^{d-1}$ *and* $\{c_r\}_{r=1}^d$ *such that:*

$$tP_r = b_{r-1}P_{r-1} + a_r P_r + c_{r+1}P_{r+1}, \qquad r = 0, 1, \dots, d-1$$

$$P_{r+1} = \frac{1}{c_{r+1}}((t - a_r)P_r - b_{r-1}P_{r-1}), \qquad r = 0, 1, \dots, d-1.$$

where we consider $P_{-1} = b_{-1} := 0$. We can compute these coefficients by

$$a_r = \frac{\langle tP_r, P_r\rangle_\sigma}{\langle P_r, P_r\rangle_\sigma}, \quad r = 0, \dots, d,$$
$$b_r = \frac{\langle tP_{r+1}, P_r\rangle_\sigma}{\langle P_r, P_r\rangle_\sigma}, \quad r = 0, \dots, d-1,$$
$$c_r = \frac{\langle tP_{r-1}, P_r\rangle_\sigma}{\langle P_r, P_r\rangle_\sigma}, \quad r = 1, \dots, d.$$

Moreover $c_{r+1}b_r > 0$, for $r \geq 0$.

Proof. The first part of the proposition was discussed before. We need to prove that $c_{r+1}b_r > 0$.

We know that $c_r \neq 0$, for $\deg(tP_r) = r+1$ and $\deg(P_{r-1}), \deg(p_r) \leq r$. We can conclude what we want by doing the division

$$\frac{b_r}{c_{r+1}} = \frac{\langle P_{r+1}, P_{r+1}\rangle_\sigma}{\langle P_r, P_r\rangle_\sigma} > 0.$$

□

Proposition 5.2 can be rewritten as a matrix multiplication:

Corollary 5.3. *The operator multiplication by t, in the basis $\{P_0, \dots, P_d\}$ is given by the following tridiagonal matrix*

$$T := \begin{pmatrix} a_0 & c_1 & & & & \\ b_0 & a_1 & c_2 & & & \\ & b_1 & a_2 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & b_{d-2} & a_{d-1} & c_d \\ & & & & b_{d-1} & a_d \end{pmatrix},$$

where the values for a_r, b_r, c_r are defined in Proposition 5.2. Moreover, the characteristic polynomial of T is $\phi = \prod(t - \lambda_r)$.

Proof. As $t^{d+1} \equiv -\tilde{\phi}$, where $\tilde{\phi} := \phi - t^{d+1}$, the multiplication by t in the standard basis $\{0, t, \dots, t^{d-1}, t^d\}$ is given by

$$\begin{pmatrix} t & t^2 & \dots & t^d & -\tilde{\phi} \end{pmatrix},$$

which is the companion matrix of ϕ and has as characteristic polynomial ϕ. Here we are using the abuse of notation

$$\sum a_r t^r \leftrightarrow \begin{pmatrix} a_0 \\ \vdots \\ a_d \end{pmatrix}.$$

□

Let $\{\tilde{P}_0, \ldots, \tilde{P}_d\}$ be another basis of orthogonal polynomials with $\deg(\tilde{P}_r) = r$. In this case, we will have non-zero constants γ_r such that $\tilde{P}_r = \gamma_r P_r$, and thus the new tridiagonal matrix, representing the multiplication by t in this new basis, will be

$$\tilde{T} = \begin{pmatrix} \tilde{a}_0 & \tilde{c}_1 & & & & \\ \tilde{b}_0 & \tilde{a}_1 & \tilde{c}_2 & & & \\ & \tilde{b}_1 & \tilde{a}_2 & \tilde{c}_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \tilde{b}_{d-2} & \tilde{a}_{d-1} & \tilde{c}_d \\ & & & & \tilde{b}_{d-1} & \tilde{a}_d \end{pmatrix}$$

$$= \Gamma T \Gamma^{-1} = \begin{pmatrix} a_0 & \frac{\gamma_0}{\gamma_1} c_1 & & & & \\ \frac{\gamma_1}{\gamma_0} b_0 & a_1 & \frac{\gamma_1}{\gamma_2} c_2 & & & \\ & \frac{\gamma_2}{\gamma_1} b_1 & a_2 & \frac{\gamma_2}{\gamma_3} c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{\gamma_{d-1}}{\gamma_{d-2}} b_{d-2} & a_{d-1} & \frac{\gamma_{d-1}}{\gamma_d} c_d \\ & & & & \frac{\gamma_d}{\gamma_{d-1}} b_{d-1} & a_d \end{pmatrix}, \qquad (*)$$

where Γ is the diagonal matrix with γ_r as entries, corresponding to the matrix of change of basis.

We observe that the diagonal of $\tilde{T}$ is the same for every orthogonal basis as well as the product of $\tilde{b}_r \tilde{c}_{r+1}$. However, with an appropriate choice of the $(\gamma_r)_r$, we can set, for each pair $(\tilde{b}_r, \tilde{c}_{r+1})$, an arbitrary non-negative number for $\tilde{b}_r$ or $\tilde{c}_{r+1}$, but once one is chosen the other is uniquely defined.

Another important observation is that when we multiply each polynomial P_r by the **same** constant, we have $\tilde{T} = T$.

Some interesting choices for $\tilde{b}_r, \tilde{c}_r$ are:

- $\tilde{c}_r = 1$ for each r, in which case the polynomials $\tilde{P}_r$ are monic;
- $\tilde{c}_{r+1} = \tilde{b}_r$ for each r. In this case $\tilde{T}$ is self-adjoint and $\|P_r\|_\sigma$ is constant in r;
- The vectors P_r are normal concerning the Euclidian norm, by doing $P_r := \tilde{P}_r / \|\tilde{P}_r\|$ for any sequence of $\tilde{P}_r$.

Now, we will consider $\mathbb{R}[t]$ instead of the quotient. We will define $c_{d+1} := 1$, $c_0 := P_0^{-1}$ and

$$P_{d+1} := (t - a_d)P_d - b_{d-1}P_{d-1}.$$

In this case, we have the following result.

Proposition 5.4. *Let $T[r]$ be the main $r \times r$-submatrix of T. Then:*

$$\left(\prod_{s=0}^{r} c_s\right) P_r = \det(tI - T[r]).$$

In particular $P_{d+1} = (\prod c_r)\,\phi$*. Moreover, the eigenvector related to* λ_r *is*

$$\xi_r := \begin{pmatrix} P_0(\lambda_r) \\ P_1(\lambda_r) \\ \vdots \\ P_d(\lambda_r) \end{pmatrix}.$$

Proof. The proof uses induction on r. The base case is true because we defined c_0 for it. For $r+1$, Lagrange's formula gives us

$$\begin{aligned} \det(tI - T[r+1]) &= (t-a_r)\det(tI - T[r]) - c_r b_{r-1}\det(tI - T[r-1]) \\ &= (t-a_r)\left(\prod_{s\le r} c_s\right) P_r - c_r b_{r-1}\left(\prod_{s\le r-1} c_s\right) P_{r-1} \\ &= \left(\prod_{s\le r} c_s\right)((t-a_r)P_r - b_{r-1}P_{r-1}) \\ &= \left(\prod_{s\le r+1} c_s\right) P_{r+1}. \end{aligned}$$

For the eigenvector, fix a λ_r and let M be the matrix whose s-th line is the vector P_s. We shall also use the identification $\sum a_r t^r = \begin{pmatrix} a_0 & a_1 & \dots & a_d \end{pmatrix}$. If we call $\Lambda = \begin{pmatrix} \lambda_r^0 & \lambda_r^1 & \dots & \lambda_r^{d-1} \end{pmatrix}^*$ we have $M\Lambda = \xi_r$. By Proposition 5.2 and its generalization, we have

$$TM = \begin{pmatrix} tP_0(t) \\ tP_1(t) \\ \dots \\ tP_d(t) - P_{d+1}(t) \end{pmatrix},$$

thus, since $P_{d+1}(\lambda_r) = 0$,

$$T\xi_r = (TM)\Lambda = \begin{pmatrix} \lambda_r P_0(\lambda_r) \\ \lambda_r P_1(\lambda_r) \\ \dots \\ \lambda_r P_d(\lambda_r) \end{pmatrix} = \lambda_r \xi_r.$$

□

5.2.1 The inverse problem

Now, we will address the converse problem: given a tridiagonal matrix T, how can we construct the polynomials $P_0, \dots, P_d$ and an inner product $\langle .,. \rangle_\sigma$ such that the matrix of multiplication by t is T in this orthogonal basis? We cannot uniquely determine all the polynomials since multiplying each P_r by a constant results in the same matrix T. Therefore, we can fix an arbitrary value for P_0. Additionally, T must satisfy the condition of having $b_r c_{r+1} > 0$ for each r since it was a requirement for the matrix T. We can still proceed with the construction even if T does not meet this condition, although in that case, we will obtain a non-positive defined bilinear form.

Starting from P_0 and T, we can use the recurrence relation on polynomials to calculate all the other polynomials P_r. Now, we want to determine the inner product for which the P_r are orthogonal and show that it can be expressed in the form

$$\langle p, q \rangle_\sigma = \sum \alpha_r p(\lambda_r) q(\lambda_r),$$

which is equivalent to the existence of a positive diagonal matrix Δ such that

$$\langle p, q \rangle_\sigma = p^* V^* \Delta V q,$$

in which case, $\alpha_r = \sqrt{\Delta_r}$.

We observe that $\langle \cdot, \cdot \rangle_\sigma$ also cannot be determined uniquely, since by scaling the inner product by a constant, $\langle \cdot, \cdot \rangle_{\sigma'} = \theta \langle \cdot, \cdot \rangle_\sigma$, we obtain the same values for a_r, b_r, c_r by Proposition 5.2. Thus, we can fix a value for it, let us say $\langle P_0, P_0 \rangle_\sigma =: \eta_0 > 0$. From that,

$$\langle P_{r+1}, P_{r+1} \rangle_\sigma = \frac{b_r}{c_{r+1}} \langle P_r, P_r \rangle_\sigma ,$$

which we use to uniquely determine all the other values of $\eta_r =: \langle P_r, P_r \rangle_\sigma$. The above equation also implies that T is symmetric iff $\eta_r = \eta_s$ for all r, s.

The inner product is already uniquely defined, for it is defined on the basis P_r by

$$\langle P_r, P_s \rangle_\sigma := \eta_r \delta_{r,s},$$

which ensures the orthogonality of the P_r.

However, we must still verify that the product will be in the desired form.

Let $P = \begin{pmatrix} P_0 & P_1 & \dots & P_d \end{pmatrix}$, using Proposition 5.4 we conclude that

$$VP = \begin{pmatrix} \xi_0^* \\ \xi_1^* \\ \vdots \\ \xi_d^* \end{pmatrix}.$$

Let D be the diagonal matrix such that DTD^{-1} is self-adjoint. If ξ_r is an eigenvector of T, then $D\xi_r$ will be an eigenvector of DTD^{-1}. Thus, the matrix $D(VP)^*$ will have as columns the eigenvectors of DTD^{-1}, which are orthogonal and thus there is a diagonal matrix H such that:

$$(D(VP)^*)^* D(VP)^* = H,$$

or, equivalently,

$$H^{-1/2}(VP)DD(VP)^*H^{-1/2} = I,$$

$$D(VP)^*H^{-1/2}H^{-1/2}(VP)D = I,$$

$$P^*V^*H^{-1}VP = D^{-2}.$$

We can see from the equation $*$ that D has only to satisfy

$$D_{r+1}^2 = \frac{c_{r+1}}{b_r}D_r^2.$$

Thus we can choose $D_r = 1/\sqrt{\eta_r}$ and set $\alpha_r = H_r^{-1}$, which concludes that the inner product is indeed of the desired form. It is also easy to calculate $H = VPD^2P^*V^*$, which gives us a matrix way of obtaining the weights α_r.

Another way to calculate α_r is to observe that by Proposition 5.4 and the Spectral Theorem, we have:

$$E_r = \frac{1}{\|\xi_r\|^2}\xi_r\xi_r^*, \qquad \sum_r E_r = I,$$

$$\left(\sum_r E_r\right)_{a,b} = \sum_r \frac{P_a(\lambda_r)P_b(\lambda_r)}{\|\xi_r\|^2} = \delta_{a,b},$$

which gives us the weights

$$\alpha_r = \frac{1}{\|\xi_r\|^2},$$

where

$$\xi_r = \begin{pmatrix} P_0(\lambda_r) \\ P_1(\lambda_r) \\ \vdots \\ P_n(\lambda_r) \end{pmatrix},$$

as expected, since the weights are the square of the values that normalize the eigenvectors ξ_r.

5.3 Interlacing

Interlacing is a fundamental concept in linear algebra that plays a crucial role in studying orthogonal polynomials. Let us begin with the basic definition:

Definition 5.5. *We say that two polynomials $p, q \in \mathbb{R}[t]$ with all real roots, $\lambda_1 \leq \cdots \leq \lambda_n$ and $\mu_1 \leq \cdots \leq \mu_m$, respectively, with $n > m$,* ***interlace*** *iff*

$$\lambda_r \leq \mu_r \leq \lambda_{n-(m-r)}, \qquad r = 1, \ldots, m.$$

Moreover, we say that they ***strictly interlace*** *if p, q are also coprime.*

The main result involving interlacing, which can be found in [9], is:

Theorem 5.6 (Cauchy interlacing)**.** *Suppose that M is a self-adjoint matrix in $\mathbb{M}_n(\mathbb{C})$ and S is a linear operator from $\mathbb{C}^m$ to $\mathbb{C}^n$, where $n > m$. Assume that $S^*S = I_m$, and call $N = S^*MS$. Then, the characteristic polynomials of M and N interlace.*

Corollary 5.7. *Let $\{P_r\}$ be an orthogonal polynomial sequence, with $\deg(P_r) = r$. For each r, P_r and P_{r+1} strictly interlace. Moreover, P_r has all roots simple.*

Proof. Theorem 5.6 with $S = \begin{pmatrix} I_r & \\ & 0_1 \end{pmatrix}$ and $M = T[r+1]$, together with Proposition 5.4, allow us to conclude that P_r and P_{r+1} interlace.

If θ is a common root of P_r and P_{r+1} then:

$$\theta P_r(\theta) = b_{r-1}P_{r-1}(\theta) + a_r P_r \theta + c_{r+1}P_{r+1}(\theta),$$

which implies that θ is a root of P_{r-1}. Thus, repeating the argument, we would have that θ is a root of P_0, a contradiction.

For the last part, we observe that if P_r has θ as a double root due to interlacing, P_{r-1} would also have θ as a root, contradicting what we have just proved. □

The following results of this section can be found in [11]:

Proposition 5.8. *Let $p, q \in \mathbb{R}[t]$, be monic coprime polynomials with real roots λ_r and μ_r, respectively. The following statements are equivalent:*

(1) p, q strictly interlace and $\deg(p) = \deg(q) + 1 = d + 1$;

(2) q/p has simple poles with positive residue;

(3) $(q/p)'(t) < 0$ $(t \in \mathbb{R}; t \neq \lambda_r)$;

(4) $(q/p)'(t) \leq 0$ $(t \in \mathbb{R}; t \neq \lambda_r)$;

(5) $(p/q)'(t) \geq 1$ $(t \in \mathbb{R}; t \neq \mu_r)$;

Proof. (1) $\implies$ (2): Given $\lambda_0 < \mu_0 < \ldots \mu_{d-1} < \lambda_d$, where λ_r are the roots of p and μ_r are the roots of q, the poles of q/p are λ_r, with residue given by

$$\left.\frac{q(t)(t-\lambda_r)}{p(t)}\right|_{t=\lambda_r}.$$

Since the roots of p are simple, p changes sign at its roots and, being monic, $p(t) > 0$ for $t > \lambda_d$. Therefore, $p(\lambda_r + \epsilon)$ is positive when r is of the form $r = d - 2s$ for some $s \in \mathbb{N}$ and is negative for the other values of r. On the other hand, a similar analysis shows that $q(\lambda_r + \epsilon) > 0$ for r of the form $r = d - 2s$ and negative for the other values.

(2) $\implies$ (3) we observe that we can write q/p as a partial fraction

$$\frac{q}{p} = \sum_r \frac{c_r}{t - \lambda_r},$$

and so

$$c_r = \operatorname{res}\left(\frac{c_r}{t-\lambda_r}, t = \lambda_r\right) = \operatorname{res}\left(\sum_s \frac{c_s}{t-\lambda_s}, t = \lambda_r\right) = \operatorname{res}\left(\frac{q}{p}, t = \lambda_r\right) > 0.$$

This equation implies

$$\left(\frac{q}{p}\right)' = \sum_s \frac{-c_s}{(t-\lambda_s)^2} < 0.$$

(4) $\implies$ (1): as q/p is non-increasing, between two poles of the function, which are the roots of p, the function must change sign. Thus, by continuity, there is zero of q/p, which corresponds to a root of q.

Now that we have proved the equivalence of $(1), (2), (3), (4)$ we move on to (5). (5) $\implies$ (4) follows from a simple calculation

$$\left(\frac{q}{p}\right)' = \left(\frac{1}{p/q}\right)' = -\frac{(p/q)'}{(p/q)^2} \leq -\frac{1}{(p/q)^2} < 0$$

For (4) $\implies$ (5), we first observe that

$$q^2\left(\frac{p}{q}\right)' = p'q - pq' = -p^2\left(\frac{q}{p}\right)'.$$

Also, we have

$$p^2\left(\frac{q}{p}\right)' = -\sum c_r \frac{p^2}{(t-\lambda_r)^2}.$$

Together with

$$q^2 = \left(\sum c_r \frac{p}{t-\lambda_r}\right)^2,$$

we obtain the following formula:

$$\left(\sum c_r \frac{p}{t-\lambda_r}\right)^2 \left(\frac{p}{q}\right)' = \sum c_r \frac{p^2}{(t-\lambda_r)^2}.$$

Since p and q are monic, we have $\sum c_r = 1$. Therefore, using Cauchy-Schwarz on $(\sqrt{c_r})_r$ and $\left(\frac{p\sqrt{c_r}}{t-\lambda_r}\right)_r$, we have

$$\left(\sum c_r \frac{p}{t-\lambda_r}\right)^2 \leq \sum c_r \frac{p^2}{(t-\lambda_r)^2},$$

from where we conclude that $(p/q)' \geq 1$. $\square$

Lemma 5.9. *If p and q are monic strictly interlacing real polynomials with degrees $d+1$ and d, respectively, and both have real roots, then there exist real numbers α and β, and a monic polynomial r of degree $d-1$, such that $\beta > 0$ and*

$$p = (t-\alpha)q - \beta r.$$

Furthermore, r and q strictly interlace.

Proof. Using Euclidean division, we can obtain unique numbers α and β, as well as a polynomial r with $\deg(r) < d$, such that $p = (t-\alpha)q - \beta r$. We aim to prove that $\beta > 0$ and r and q interlace.

Dividing by q we obtain

$$\frac{p}{q} = t - \alpha - \beta\frac{r}{q},$$

which implies

$$\beta\left(\frac{r}{q}\right)' = 1 - \left(\frac{p}{q}\right)'.$$

Since we know that $(p/q)' \geq 1$, we have $\beta(r/q)' \leq 0$. As $(r/q)'(t) < 0$ for large t, we can conclude that $\beta > 0$ and $(r/q)' \leq 0$ where it is defined. Therefore, as $\gcd(r,q) = \gcd(p,q) = 1$, we can apply the equivalence in Proposition 5.8 to conclude what we want. □

This lemma allows us to conclude the following result, which will be useful later:

Proposition 5.10. *If p and q are monic strictly interlacing polynomials of degree $d+1$ and d, respectively, there exists a unique sequence of monic polynomials $P_0 = 1, P_1, \dots, P_{d-1}$ with increasing degree and an inner product on $\mathbb{R}^{d+2}$ such that $P_0, P_1, \dots, P_{d-1}, q, p$ are orthogonal polynomials.*

Proof. Based on what we have seen, our goal is to find numbers a_r and b_r, with $b_r > 0$, that satisfy Proposition 5.2, where we define $c_r = 1$ as we are demanding all polynomials to be monic.

Using Lemma 5.9, we can write $p = (t-\alpha)q - \beta r$, where r is a polynomial of degree $d-1$ and α and β are unique numbers. Then we define $a_d := \alpha$, $b_{d-1} := \beta$, and $P_{d-1} := r$. Since q and r interlace and $\deg(r) = d-1$, we can continue the process and obtain all the values of a_r and b_r □

It is important to note that Proposition 5.10 provides us with an algorithm to construct the entire chain of polynomials rather than just establishing the existence of a sequence.

An immediate consequence of this proposition, along with Theorem 5.6 and Proposition 5.4, is that Lemma 5.9 is, in fact, an equivalent condition for interlacing.

If q is the characteristic polynomial of a submatrix with characteristic polynomial p, then p, q interlace by Theorem 5.6. However, if the matrix is tridiagonal, we can ensure stronger conditions, such as the interlacing being strict, as seen in Corollary 5.7. Another interlacing characteristic that is guaranteed by the matrix being tridiagonal is the following:

Definition 5.11. *Two polynomials p and q and $\deg(q) < \deg(p)$, **strongly interlace** they have real simple roots, and there exists at least one root of p in any closed interval with extremities in two distinct roots of q.*

This result is due to [4]:

Proposition 5.12. *If a sequence of orthogonal polynomials with increasing degree contains p, q, then p, q strongly interlace.*

Proof. Without loss of generality, we can assume that $\deg(p) = d + 1$ and that the inner product is supported on its roots. Let us suppose that for two roots of q, μ_1, μ_2, there is no root λ_r of p. In this case, let us call

$$\tilde{q} := \frac{q}{(t - \mu_1)(t - \mu_2)}.$$

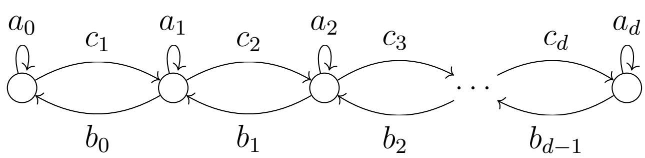
As $\deg(\tilde{q}) < \deg(q)$ they must be orthogonal, hence

$$0 = \langle q, \tilde{q} \rangle_\sigma = \sum \alpha_r \frac{q^2(\lambda_r)}{(\lambda_r - \mu_1)(\lambda_r - \mu_2)},$$

for some constants $\alpha_r > 0$. Well, since there is no λ_r in between μ_1 and μ_2, the sign of $\lambda_r - \mu_1$ and $\lambda_r - \mu_2$ must must be constant for all r. Thus, the sum on the right side is strictly positive, which leads to a contradiction. □

5.4 Weighted paths

In this chapter, we shall describe the occurrence of PST on positive-weighted path digraphs, possibly with loops. A general weighted path is of the form



and its adjacency matrix is

$$A(X) = \begin{pmatrix} a_0 & c_1 & & & & \\ b_0 & a_1 & c_2 & & & \\ & b_1 & a_2 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & b_{d-2} & a_{d-1} & c_d \\ & & & & b_{d-1} & a_d \end{pmatrix}.$$

We observe that for each positive tridiagonal matrix A, we have a weighted graph whose adjacency matrix is A. This gives us a bijection between these two objects.

We can perform some arithmetical operations on the adjacency with PST, which maintains the PST. As a result, we can assume that the graphs possess certain favorable properties, as we can reconstruct graphs with these properties by performing operations on well-behaved graphs.

Firstly, as $e^{it(\alpha T)} = e^{i(t\alpha)T}$, we have PST in T iff we have one in αT, and also we have

$$|(e^{it(\mu I+T)})_{a,b}| = |(e^{it\mu} I e^{itT})_{a,b}| = |e^{it\mu}| \cdot |(e^{itT})_{a,b}| = |(e^{itT})_{a,b}|,$$

that is, we can sum μI without changing the existence of PST.

That allows us to suppose that two eigenvalues are integers without loss of generality. Thus, we can also suppose that all the spectra are integers since we must have the ratio condition on the eigenvalue support by Proposition 3.6. We can also suppose that the spectrum has the greatest common divisor 1; otherwise, we can divide the whole matrix by its greatest common divisor.

5.4.1 First case: PST between extremities

This subsection is motivated by [27].

When do we have PST between the extremities of the weighted path associated with T?

The first step is to analyze cospectrality, which is done by the following theorem:

Theorem 5.13. *Let T be a tridiagonal self-adjoint matrix with positive off-diagonal elements, and $\tilde{P}_r$ be the associated orthogonal monic polynomials obtained by*

$$\tilde{P}_r := \det(tI - T[r]), \quad P_0 = 1.$$

Denote

$$R := \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & \iddots & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix}.$$

Then the following are equivalent:

(1) The first and last vertices of the related path are strongly-cospectral;

(2) Each vertex of the related path is strongly cospectral to its opposite vertex;

(3) $[T, R] = 0$*;*

(4) $\tilde{P}_d(\lambda_r) = (-1)^{d-r}$.

Proof. We show that (1) $\implies$ (3). Let us designate the first and last vertices as x and y, respectively. We want to show that $a_r = a_{d-r}$ and $b_r = b_{d-r-1}$, which is equivalent to $[T, R] = 0$. The number of 1-cycles in x is given by a_0, and in y it is counted by a_d. Therefore, we have $a_0 = a_d$. Similarly, the number of 2-cycles in x is $c_1 + b_0 + a_0^2 = 2b_0 + a_0^2$, and in y it is $2b_{d-1} + a_d^2$, from where and $b_0 = b_{d-1}$.

Now, let us consider the absurd case where $b_k > b_{d-k}$, and let k be the smallest value that satisfies this condition. Additionally, assume that $a_r = a_{d-r}$ for all $r \leq k$. In this scenario, the total weight of the $(2k)$-cycles starting at x would be greater because we would have the same cycles as in y, each with exactly the same weight except for the weight of b_k. Similarly, if $a_k > a_{d-k}$ and $a_r = a_{d-r}$ and $b_r = b_{d-r}$ for all $r < k$, we would observe a greater total weight on the $(2k+1)$-cycles starting at x. A similar argument can be applied for the other cases when $b_k < b_{d-k}$ or $a_k < a_{d-k}$.

Now, for (3) $\implies$ (2), we observe that as T has simple eigenvalues we have $[T, R] = 0$ iff there is a polynomial p such that $p(T) = R$. Thus, we will have $P(A)e_r = Re_r = e_{d-r}$, and (6) of Theorem 2.24 ensure us that e_r and e_{d-r} are strongly cospectral.

For (4) $\iff$ (1), we first recall that Proposition 5.4 gives us

$$(E_r)_{a,b} = \frac{P_a(\lambda_r)P_b(\lambda_r)}{\|\xi_r\|^2},$$

where

$$\xi_r := \begin{pmatrix} P_0(\lambda_r) \\ P_1(\lambda_r) \\ \vdots \\ P_d(\lambda_r) \end{pmatrix},$$

and P_r is the normalized orthogonal polynomial, defined by $P_r := (\prod_{s=1}^{r} c_s)\tilde{P}_r$.

Now, item (1) Theorem 2.24, tells us that we have (4) iff

$$(E_r)_{0,0} = (E_r)_{d,d},$$

which happens iff

$$\frac{P_0(\lambda_r)^2}{\|\xi_r\|^2} = \frac{P_d(\lambda_r)^2}{\|\xi_r\|^2},$$

or, equivalently

$$P_d(\lambda_r)^2 = P_0(\lambda_r)^2 = 1.$$

The fact that P_d has real zeros and $|P_d(\lambda_r)| = 1$ implies that $P_d(\lambda_r) = (-1)^{d-r}$. □

Now let us call $0, d$ the first and last vertex of the weighted path, respectively. We shall now revisit Theorem 3.10 and see the conditions for having PST between 0 and d. As

$$(E_r)_{0,0} = \frac{P_0(\lambda_r)P_0(\lambda_r)}{\|\xi_r\|^2} = \frac{1}{\|\xi_r\|^2} > 0,$$

we see that the eigenvalue support of 0 is all the spectrum. Thus, to have condition (2), we can assume without loss of generality that the spectrum is integer and coprime. Now, for condition (3) we have

$$(E_r)_{0,d} = \frac{P_0(\lambda_r)P_d(\lambda_r)}{\|\xi_r\|^2} = \frac{(-1)^{d-r}}{\|\xi_r\|^2}.$$

Hence, λ_r must be alternating between odd and even. This way, we have an algorithm to generate all the weighted paths with PST between the extremities, given by:

Theorem 5.14. *The following algorithm generates all possible matrices of weighted $(d+1)$-paths whose extremities have PST:*

(1) Choose $d{+}1$ distinct integers (your favorite ones!) $\lambda_0 < \cdots < \lambda_d$, where $\lambda_r \equiv r \mod 2$;

(2) Define P_d as the polynomial of degree d such that $P_d(\lambda_r) = (-1)^{d-r}$;

(3) Call $\tilde{P}_d$ be the monic polynomial associated with P_d;

(4) Calculate $\tilde{P}_{d-1}, \ldots, \tilde{P}_1, \tilde{P}_0$ using the algorithm in Proposition 5.10;

(5) Calculate the values a_r, b_r and construct a matrix $\tilde{T}$ (we already have $c_r = 1$);

(6) Let T be the symmetric matrix obtained by conjugating $\tilde{T}$ by a diagonal (or by using $b_r = c_{r+1} = \sqrt{\tilde{b}_r}$);

(7) We may do operations of the form $T + \beta I$ or αT for $\alpha, \beta \in \mathbb{R}$.

A natural question is whether there are other vertices with PST in a weighted path with PST between extremities. The answer is positive:

Proposition 5.15. *If there is PST between the extremities of a weighted path in time τ, then there is PST at time τ for any pair of symmetrical vertices.*

Proof. We postpone the proof to after Proposition 5.16. □

5.4.2 Orthogonal polynomial sequence with fixed terms

This subsection is a generalization of the results from the previous one and is made mainly of the original results that we obtained in our research.

Suppose we aim to achieve PST between vertices 0 and $d-k$ in the $d+1$ path. We begin by assuming that we have the orthogonal polynomial is associated with the vertex, denoted as P_{d-k}. We want to determine the properties that P_{d-k} must possess in order to be part of a chain of d orthogonal polynomials, ensuring PST between 0 and $d-k$, and also recover a sequence of orthogonal polynomials which contains both P_{d-k} and P_{d+1} as a last polynomial. We will approach the former task. We begin with the following propositions, likely known in the theory, which establish a relationship between the values of P_d and P_{d-k}. However, we could not find a reference, and the proof we present is due to the author.

Proposition 5.16. *Let $P_0, \dots, P_d$ be a sequence of monic orthogonal polynomials of increasing degree, with inner product supported on the roots of P_{d+1}, also monic. Then, for any $0 \leq k \leq d$, if P_{d-k} does not share any root with P_{d+1}, we have:*

$$\frac{P_d}{P_{d+1}} = \sum_{r=0}^{d} \left(\prod_{s=d-k}^{d-1} b_s \right) \frac{P_{d-k}(\lambda_r)}{\phi_k(\lambda_r)} \cdot \frac{1}{\prod_{s \neq r}(\lambda_r - \lambda_s)} \cdot \frac{1}{(t-\lambda_r)},$$

where

$$A_k := \begin{pmatrix} a_{d-k+1} & 1 & & \\ b_{d-k+1} & a_{d-k+1} & & \\ & & \ddots & 1 \\ & & b_{d-1} & a_d \end{pmatrix}, \qquad \phi_k(t) := \det(tI - A_k), \ \phi_0 := 1.$$

Proof. We start by noticing that by multiplying both sides by P_{d+1}, we obtain that the formula is equivalent to

$$P_d = \sum_{j=0}^{d} \frac{\left(\prod_{s=d-k}^{d-1} b_s\right) P_{d-k}(\lambda_j)}{\phi_k(\lambda_j)} \cdot \frac{\prod_{s \neq j}(t-\lambda_s)}{\prod_{s \neq j}(\lambda_j - \lambda_s)}.$$

Since both sides of the equation are polynomials of degree d, we can prove equality by showing that they are equal for the $d+1$ values of λ_j. Thus, by setting $t = \lambda_r$, we can eliminate all terms in the sum except for the one where $j = r$, giving us

$$P_d(\lambda_r) = \frac{\left(\prod_{s=d-k}^{d-1} b_s\right) P_{d-k}(\lambda_r)}{\phi_k(\lambda_r)}.$$

The equation can be rewritten as:

$$P_d(\lambda_r)\phi_k(\lambda_r) = \left(\prod_{s=d-k}^{d-1} b_s\right) P_{d-k}(\lambda_r). \tag{$**$}$$

We will prove ($**$) by induction on k. First, it is easy to see that for $k = 1$, ($**$) is

$$(\lambda_r - a_d)P_d(\lambda_r) = b_{d-1}P_{d-1}(\lambda_r),$$

which is true since

$$(t - a_d)P_d - b_{d-1}P_{d-1} = P_{d+1},$$

and the roots of P_{d+1} are precisely λ_r. For $k = 0$, we defined $\phi_0 := 1$. With that, ($**$) is satisfied.

For the induction, we note that by Lagrange's formula, we have:

$$\phi_k = (t - a_{d-k+1})\phi_{k-1} - b_{d-k+1}\phi_{k-2}, \qquad k \geq 2.$$

Additionally, we can use the recursion relation given in Proposition 5.2 to obtain:

$$b_{d-k}P_{d-k} = (t - a_{d-k+1})P_{d-k+1} - P_{d-(k-2)}, \qquad k \geq 2.$$

Now, by doing some manipulation:

$$\begin{aligned}
\left(\prod_{s=d-k}^{d-1} b_s\right) P_{d-k}(\lambda_r) &= \left(\prod_{s=d-(k-1)}^{d-1} b_s\right) b_{d-k}P_{d-k}(\lambda_r) \\
&= \left(\prod_{s=d-(k-1)}^{d-1} b_s\right) \big((t - a_{d-k+1})P_{d-k+1} - P_{d-(k-2)}\big) \\
&= (\lambda_r - a_{d-(k-1)})P_d(\lambda_r)\phi_{k-1}(\lambda_r) - b_{d-(k-1)}P_d(\lambda_r)\phi_{k-2}(\lambda_r) \\
&= P_d(\lambda_r)\left((\lambda_r - a_{d-(k-1)})\phi_{k-1}(\lambda_r) - b_{d-(k-1)}\phi_{k-2}(\lambda_r)\right) \\
&= P_d(\lambda_r)\phi_k(\lambda_r)
\end{aligned}$$

□

Proof of Proposition 5.15. We already have the condition (2) of Theorem 3.10 on the eigenvalues and, by Theorem 5.13 cospectrality between vertices $d - k$ and k. The same proposition also implies that $\phi_r = P_r$. We can use ($**$) regardless of having distinct zeroes of the polynomials, and using this formula, we conclude:

$$\begin{aligned}
(E_r)_{k,d-k} &= \alpha P_k(\lambda_r)P_{d-k}(\lambda_r) \\
&= (\alpha\beta)P_d(\lambda_r)\phi_{d-k}(\lambda_r)P_{d-k}(\lambda_r) \\
&= (\alpha\beta)P_{d-k}(\lambda_r)^2 P_d(\lambda_r)
\end{aligned}$$

where $\alpha = \left(\sum_s P_s(\lambda_r)^2\right)^{-1} > 0$ and $\beta = \left(\prod_{s=d-k}^{d-1} b_s\right)^{-1} > 0$. This equality allows us to conclude that $(E_r)_{k,d-k}$ and $P_d(\lambda_r)$ have the same sign in the spectral support of the vertex, which is equivalent to condition (3) of Theorem 3.10 for k and $d - k$. □

The next two results are derived from the application of Proposition 5.16. The accompanying proofs are original and likely contribute novel insights to the theory.

Theorem 5.17. *Suppose P_{d-k} and P_{d+1} are monic, coprime, strongly interlacing polynomials of degrees $d-k$ and $d+1$, respectively. Call λ_r the roots of P_{d+1}. Let $a_{d-k+1}, \dots, a_d$ and $b_{d-k+1}, \dots, b_{d-1}$ be sequences of real numbers, with $b_r > 0$.*

Then, there exists a sequence of orthogonal monic polynomials $P_0, \dots, P_d$ with respect to a measure supported on the roots of P_{d+1}, and with corresponding coefficients a_r and b_r, iff each interval $(\lambda_r, \lambda_{r+1})$ of roots of P_{d+1} which does not contain a root of P_{d-k} has a root of ϕ_k, which is defined as in Proposition 5.16.

Proof. The condition on the zeros is equivalent to having $P_{d-k}\phi_k$ and P_{d+1} coprimes and interlacing. We observe that a sequence of orthogonal polynomials exists iff the value of P_d defined by Proposition 5.16 interlaces P_{d+1} since, in this case, we can define P_d by these values and reconstruct the whole sequence using Proposition 5.10. The sequence derived from P_d and P_{d+1} must contain P_{d-k}, since its polynomial of degree $d-k$ has the same value at the points λ_r, by another use of 5.16.

By Proposition 5.8, P_d interlacing P_{d+1} is equivalent to

$$\operatorname{res}\left(\frac{P_d(t)}{P_{d+1}(t)}, t = \lambda_r\right) > 0, \qquad \forall r,$$

which means

$$\frac{\left(\prod_{s=d-k}^{d-1} b_s\right) P_{d-k}(\lambda_r)}{\phi_k(\lambda_r)} \cdot \frac{1}{\prod_{s\neq r}(\lambda_r - \lambda_s)} > 0.$$

Notably, dividing both sides by $\prod b_s$ does not affect the sign of the term since $b_r > 0$. We can also multiply both sides by $\phi_k(\lambda_r)^2$ without changing the inequality. The value $\phi_k(\lambda_r)$ is not zero by 5.16 and $P_{d-k}(\lambda_r) \neq 0$. This means that the above inequality is equivalent to

$$\frac{P_{k-d}(\lambda_r)\phi_k(\lambda_r)}{\prod_{s\neq r}(\lambda_r - \lambda_s)} > 0.$$

By hypothesis $P_{d-k}(t)\phi_k(t)$ interlaces P_{d+1}. Thus, by Proposition 5.8

$$\operatorname{res}\left(\frac{P_{d-k}(t)\phi_k(t)}{P_{d+1}(t)}, t = \lambda_r\right) > 0,$$

which concludes what we wanted since

$$\frac{P_{k-d}(\lambda_r)\phi_k(\lambda_r)}{\prod_{s\neq r}(\lambda_r - \lambda_s)} = \operatorname{res}\left(\frac{P_{d-k}(t)\phi_k(t)}{P_{d+1}(t)}, t = \lambda_r\right).$$

□

Let $\beta := \prod_{s=d-k}^{d-1} b_s$. We observe that β is uniquely defined by P_{d-k} and ϕ_k since there is only one value that makes the polynomial obtained by interlacing,

$$P_d = \sum_{j=0}^{d} \frac{\beta P_{d-k}(\lambda_j)}{\phi_k(\lambda_r)} \cdot \frac{\prod_{s\neq j}(t-\lambda_s)}{\prod_{s\neq j}(\lambda_j-\lambda_s)},$$

monic. So, given a ϕ_k that satisfies Theorem 5.17, we can algorithmically restore the sequence of orthogonal polynomials:

Theorem 5.18. *Let P_{d-k} and P_{d+1} be monic coprime strongly interlacing polynomials. Also, suppose they have degrees $d-k$ and $d+1$, respectively. Then a sequence of orthogonal monic polynomials $P_0, \ldots, P_d$ contains P_{d-k}, whose inner product is supported on the roots of P_{d+1}. We can create such a sequence following these steps*

(1) Choose k values $\mu_0, \ldots, \mu_{k-1}$ that lie in distinct intervals between two adjacent roots of P_{d+1} between which there are no roots of P_{d-k}. (We note that this can only be done if P_{d+1} and P_{d-k} strongly interlace);

(2) Let $\phi_k := \prod_{r=0}^{k-1}(t-\mu_r)$;

(3) Call

$$\tilde{P}_d = \sum_{j=0}^{d} \frac{P_{d-k}(\lambda_j)}{\phi_k(\lambda_j)} \cdot \frac{\prod_{s\neq j}(t-\lambda_s)}{\prod_{s\neq j}(\lambda_j-\lambda_s)},$$

and P_d the monic polynomial multiple of $\tilde{P}_d$.

(4) Obtain the remaining values of $P_0, \ldots, P_{d-1}$ by applying the procedure in Proposition 5.10 to P_d and P_{d+1}.

Moreover, these steps cover all the possible ways of forming such a sequence of orthogonal polynomials.

Corollary 5.19. *If p and q are coprime polynomials that strongly interlace and do not share common roots, then an orthogonal polynomial sequence contains both.*

The additional hypothesis of P_{d-k} and P_{d+1} not having roots in common is not a problem when we want to force PST between vertices 0 and $d-k$. Using that $(E_r)_{d-k,d-k} = P_a(\lambda_r)^2/\|\xi_r\|^2$, we conclude that λ_r is in the support of $d-k$ iff $P_{d-k}(\lambda_r) \neq 0$. Hence, as $P_0(\lambda_r) = 1 \neq 0$, we also must have $P_{d-k}(\lambda_r) \neq 0$ if there is PST.

Corollary 5.20. *Let $P_{d-k}, P_{d-l}, P_{d+1}$ polynomials with all real distinct roots and of degree $d-k, d-l$ and $d+1$ respectively, such that $\gcd(P_{d-k}, P_{d+1}) = \gcd(P_{d-l}, P_{d+1}) = 1$. Then, there exists a sequence of orthogonal polynomials containing P_{d-k} and P_{d-j} with the inner product supported on the roots of P_{d+1} iff there are polynomials ϕ_k, ϕ_l of degree k, l respectively such that*

(i) $\phi_k P_{d-k}$ and $\phi_l P_{d-l}$ interlace P_{d+1};

(ii) There is a constant c for which $\dfrac{P_{d-k}(\lambda_r)}{\phi_k(\lambda_r)} = c\dfrac{P_{d-l}(\lambda_r)}{\phi_l(\lambda_r)}$ *for each λ_r root of P_{d+1};*

Proof. Both P_{d-k} and P_{d-l} are in an orthogonal polynomial sequence with the last term, respectively,

$$P_d = \sum_{r=0}^{d} \frac{\beta P_{d-k}(\lambda_r)}{\phi_k(\lambda_r)} \cdot \frac{\prod_{s\neq r}(t-\lambda_s)}{\prod_{s\neq r}(\lambda_r-\lambda_s)}, \quad \tilde{P}_d = \sum_{r=0}^{d} \frac{\beta' P_{d-l}(\lambda_r)}{\phi_l(\lambda_r)} \cdot \frac{\prod_{s\neq r}(t-\lambda_s)}{\prod_{s\neq r}(\lambda_r-\lambda_s)},$$

for suitable constants β, β'. By (*ii*), we conclude that P_d and $\tilde{P}_d$ are scalar multiples, but since they are both monic, they must be equal. Hence, they determine the same orthogonal polynomial sequence, which contains both P_{d-k} and P_{d-l}. □

We can implement the last corollary as linear restrictions over vectors. We define the variables $x_r := \phi_k(\lambda_r)$ and $y_r := \phi_l(\lambda_r)$. The second condition now becomes the linear restriction:

$$a_r x_r = b_r y_r, \quad \forall r,$$

where $a_r := 1/P_{d-k}(\lambda_r)$ and $b_r := 1/P_{d-l}(\lambda_r)$ are given parameters.

The interlacing condition can be replaced by the demanding that x_r, y_r have adequate signs: $x_r x_{r+1} < 0$ iff there is a root of ϕ_k in $(\lambda_r, \lambda_{r+1})$ iff there are no roots of P_{d-k} in $(\lambda_r, \lambda_{r+1})$. We can write that as

$$a_r a_{r+1} x_r x_{r+1} < 0, \quad r = 1, \ldots, d-1.$$

We do not need to impose this for y_r since it will result from the other two restrictions. We also want $\deg(\phi_k) = k$, which can be checked by using interpolation and computing the unique polynomial with degrees lesser than $d+1$ that assume the values of x_r at λ_r. Similarly for $\deg(\phi_l) = l$.

We can apply Theorem 3.10 to establish conditions for having PST between vertices 0 and $d-k$ in a weighted path. Condition (1) is equivalent to having $|P_{d-k}(\lambda_r)| = 1$ for each r, by Lemma 5.22, which will be proved in the next section.

Condition (2) depends uniquely on the eigenvalue support of the vertices, which is composed of integers by hypothesis. As for condition (3), we have

$$\begin{cases} \|\lambda_0 - \lambda_r\|_2 \leq \frac{1}{2} & \lambda_r \equiv \lambda_0 \mod 2 \\ \|\lambda_0 - \lambda_r\|_2 = 1 & \lambda_r \not\equiv \lambda_0 \mod 2. \end{cases}$$

We now observe that

$$(E_r)_{0,d-k} = \frac{P_0(\lambda_r)P_{d-k}(\lambda_r)}{\|\xi_r\|^2},$$

which has the same sign as $P_{d-k}(\lambda_r)$. Thus, we have conditions (1) and (3) iff $P_{d-k}(\lambda_r) = (-1)^{\lambda_r - \lambda_0}$. This restriction leads us to the following problem involving polynomials:

Problem 5.1. *Given k, d positive integers, with $k \geq d/2$, which sequences of d integers (if any) $\lambda_0 > \lambda_1 > \cdots > \lambda_d$ and a polynomial P_{d-k} satisfy:*

(1) $\deg(P_{d-k}) = d - k$;

(2) $P_{d-k}(\lambda_r) = (-1)^{\lambda_r - \lambda_0}$,

(3) P_{d-k} *strongly interlaces* $\lambda_0, \ldots, \lambda_d$;

(4) all roots of P_{d-k} *are real.*

For each choice of value for λ_r, the polynomial P_{d-k} is uniquely defined by (2). However, the polynomial defined for an arbitrary sequence will not always have the right degree nor satisfy (3) and (4).

We summarize the discussion in this section with a result similar to Theorem 5.14:

Theorem 5.21. *The following steps generates all possible matrices of weighted d-paths with PST between vertices 0 and $d - k$:*

(1) Choose λ_r as in Problem 5.1;

(2) Compute the polynomial $\tilde{P}_{d-k}$ which satisfies the conditions of Problem 5.1;

(3) Calculate $\tilde{P}_d, \ldots, \tilde{P}_1, \tilde{P}_0$ using Theorem 5.18;

(4) Calculate the values $\tilde{a}_r, \tilde{b}_r$ and construct a matrix $\tilde{T}$ (we already have $\tilde{c}_r = 1$);

(5) Let T be the symmetric matrix obtained by conjugating $\tilde{T}$ by a diagonal (or by using $b_r = c_{r+1} = \sqrt{\tilde{b}_r}$);

(6) We may do operations of the form $T + \beta I$ or αT for $\alpha, \beta \in \mathbb{R}$.

5.4.3 Cospectrality in weighted paths

In this section, our focus shifts to a related yet somewhat weaker problem involving two cospectral vertices within a weighted path. We initiate this discussion by establishing a connection between cospectrality and orthogonal polynomials:

Lemma 5.22. *Given a weighted path, the vertices a, b are cospectral iff*

$$|P_a(\lambda_r)| = |P_b(\lambda_r)|, \qquad \forall r,$$

where P_r are the orthogonal monic polynomials related to the adjacency symmetric graph T.

Proof. Using 2.14, a, b are cospectral iff $(E_r)_{a,a} = (E_r)_{b,b}$. The result follows from $(E_r)_{a,b} = (1/\|\xi_r\|^2)P_a(\lambda_r)P_b(\lambda_r)$. □

The following corollary is a known but unpublished result of Coutinho and Spier. Nevertheless, this proof is originally ours.

Corollary 5.23. *No pair of cospectral vertices are on the same half of a weighted-path graph. The half includes the middle vertex when the path is odd.*

Proof. We have a, b cospectral iff $P_{d+1} \mid P_a^2 - P_b^2$, from where

$$d + 1 = \deg(P_{d+1}) \leq \deg(P_a^2 - P_b^2) = 2\max\{a, b\}.$$

Thus, we conclude that $\max\{a, b\} > d/2$. That is, at least one vertex is in $(d/2, d]$. We cannot have both vertices in $[d/2, d]$; otherwise, a reflection of the path would give us a path with two cospectral vertices in $[0, d/2]$. □

Corollary 5.24. *No three vertices are cospectral to each other in a weighted graph.*

Corollary 5.24 is a particular case of a stronger result: there is no tree with three cospectral vertices [12].

The following lemma generalizes Lemma 5.22 when we are dealing with non-normalized orthogonal polynomial sequences. It is particularly useful when computing the related monic orthogonal polynomials.

Lemma 5.25. *Given a sequence of orthogonal polynomials $P_0, \ldots, P_d$ we have the vertices a, b are cospectral in the symmetrized matrix $\tilde{T}$ related to these polynomials iff there is a constant $c > 0$ such that*

$$|P_a(\lambda_r)| = c|P_b(\lambda_r)|, \qquad \forall r.$$

Proof. Let $\tilde{P}_r$ denote the polynomial sequence related to the symmetrized matrix. We want to show that $P_a(\lambda_r)^2 = P_b(\lambda_r)^2$. We observe that there are constants k_1, k_2 such that $P_a = k_1\tilde{P}_a$ and $P_b = k_2\tilde{P}_b$. From that we have $\tilde{P}_a(\lambda_r)^2 = k^2\tilde{P}_b(\lambda_r)^2$ and in particular

$$\sum \frac{1}{\|\xi_r\|^2}\tilde{P}_a(\lambda_r)^2 = k^2 \sum \frac{1}{\|\xi_r\|^2}\tilde{P}_b(\lambda_r),$$

where $k = ck_2/k_1$. As $\sum \frac{1}{\|\xi_r\|^2}\tilde{P}_a(\lambda_r)^2 = \sum \frac{1}{\|\xi_r\|^2}\tilde{P}_b(\lambda_r) = 1$ we conclude that $k = 1$. □

5.5 Conclusions

In this chapter, we studied orthogonal polynomials, focused on the finite dimension space case, and how they are related to tridiagonal matrices and path graphs. We were motivated by the goal of finding PST in weighted paths since a path is the most efficient way of creating a graph with the greatest diameter with a fixed number of vertices. As there is no PST in regular paths, it was natural to study weighted paths and the theory of orthogonal polynomials, which allowed us to provide a precise interpretation of the quantum walk phenomenon. We proved an original result concerning how to create an orthogonal polynomial sequence when given a term in the middle and the last one and formulated clearly an open problem about the existence of polynomials for whose related weighted path has PST between non-extremal vertices. We point out that this problem has a connection to the Prouhet-Tarry-Escott problem [6], as forcing the polynomials to have small degrees and interpolate integer points can be rewritten as finding two multi-set integers whose powers sums are equal; as is shown in [6].

In the next chapter, we focus on the second task we induced earlier: recovering simple graphs that preserve quantum walk properties of weighted paths.

Chapter 6

Equitable partitions

Now that we have researched the problem of achieving PST in weighted graphs, we are faced with another challenge: how can we construct a simple graph that exhibits a similar quantum walk to the original weighted graph? To tackle this question, we will delve into the study of equitable partitions and quotient graphs.

While their connection to PST is established in Proposition 6.7, equitable partitions hold intrinsic value as a tool in graph theory.

Graphs with a certain degree of regularity possess particular partitions known as equitable partitions. By utilizing a graph and its equitable partition, we can define a new weighted graph called the symmetrized quotient graph. In various cases, this quotient graph retains desired properties, including PST. Section 6.1 will define these concepts and prove properties preserved in the quotient based on results and definitions from [11].

In 6.2, we will face the problem of determining the class of graphs that can be quotiented into a given graph. We will characterize in matrix terms all graphs with some quotient in common with an original theorem and compare this to the already-known theory for another type of quotient, which can be found in [25], leading us also to examine the structure that all the equitable partitions of a given graph exhibit.

In Sections 6.3 and 6.4, we focus on the inverse problem: given a graph, can we determine another graph with the original one as a quotient? For this task, we use results from [21]. While Section 6.3 presents general results, in the latter section, we explore how to compute such graphs for a given path, which is particularly interesting to us.

6.1 Preliminary definitions

The definitions and results from this section are based on [11,18]. Let us start this section by introducing a fundamental definition:

Definition 6.1. *A partition of the vertex set of a graph X is a function $\pi\colon V(X) \to [0,\dots,k-1]$. The set $C_r := \pi^{-1}(r)$ is called a cell of the partition, and we call the*

characteristic matrix of the partition *the related* $|V(X)| \times k$ *matrix* $\tilde{S}$ *defined by*

$$\tilde{S}_{ar} = \begin{cases} 1, & \pi(a) = r \\ 0, & \pi(a) \neq r \end{cases}.$$

The ***normalized characteristic matrix****,* S*, is obtained by scaling each column of* $\tilde{S}$ *such that their norm is* 1*.*

We have

$$S^* S = I_{|\pi|},$$

and since SS^* is idempotent, it must be the orthogonal projector onto $\operatorname{col} SS^* = \operatorname{col} S = \operatorname{col} \tilde{S}$, which is the space of vectors with constant coordinates on the cells of π.

Definition 6.2. *We say that a partition* π *of* X *is* ***equitable*** *iff* $N(a, C_r)$*, (the number of neighbors of* a *in* C_r*) depends only on* r *and* $\pi(a)$*, that is*

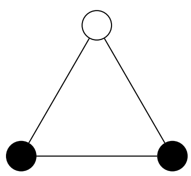
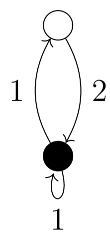
$$\forall r, s \quad a, b \in C_r \implies N(a, C_s) = N(b, C_s).$$

We note that we may have $r = s$*.*

Given an equitable partition π of X, we can define the quotient $\widetilde{X/\pi}$ as the directed graph on the cells of π where the number of arcs from r to s is equal to the number of neighbors that a vertex of C_r has in C_s. If we denote by B the adjacency matrix of $\widetilde{X/\pi}$ then

$$B_{rs} = N(a, C_s) = \frac{N(C_r, C_s)}{|C_r|} = \sum_k A_{ak} \tilde{S}_{ks}, \qquad \text{for any } a \in C_r\ .$$

The triangle has an equitable partition. We will represent different classes with different colors in the graphs. One of the triangle's equitable partitions and its related quotients and matrices are

$X =$  $\widetilde{X/\pi} =$ 

$$\tilde{S} = \begin{pmatrix} 1 & \\ & 1 \\ & 1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & \\ & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

This way, we have

$$A\tilde{S} = \tilde{S}B.$$

Lemma 6.3. *Let* π *be a partition of* X *with characteristic matrix* $\tilde{S}$ *and normalized matrix* S*. The following are equivalent:*

(1) π *is equitable;*

(2) $\operatorname{col}\tilde{S}$ *is A-invariant;*

(3) A *and* SS^* *commute.*

Proof. We start by showing $(i) \iff (ii)$. Note that the space of vectors $\operatorname{col}\tilde{S}$ is composed of the elements that are constant on the cells of π. Hence, using the fact that $(A\chi_{C_r})_a = N(a, C_r)$, we conclude that $\chi_{C_r} \in \operatorname{col}\tilde{S}$ for each r iff π is equitable. For $(2) \iff (3)$, since SS^* is a projector onto $\operatorname{col}\tilde{S}$, A and SS^* commute iff the range of A is a subspace of $\operatorname{col}\tilde{S}$, which is equivalent to $\operatorname{col}\tilde{S}$ being an A-invariant subspace. □

We note that $A\left(\widetilde{X/\pi}\right)$ is not necessarily self-adjoint, which leads us to define a new matrix related to π.

Definition 6.4. *We define the* ***symmetrized quotient graph*** *of* X *relative to* π*, denoted by* X/π*, as the graph whose adjacency matrix is*

$$C := S^*AS,$$

where A *is the adjacency matrix of* X *and* S *is the normalized characteristic matrix related to* π*.*

Equivalently, we can define the symmetrized quotient graph as the weighted graph on the cells of π *where* e_{rs} *has weight* $\sqrt{B_{rs}B_{sr}}$*, or, likewise*

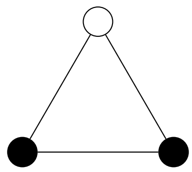
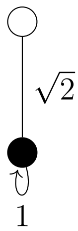
$$C_{rs} := \frac{N(C_r, C_s)}{\sqrt{|C_r||C_s|}}.$$

Here we are denoting

$$N(C_r, C_s) := \sum_{a \in C_r} N(a, C_s) = \chi_{C_r}^* A \chi_{C_s},$$

which is the number of edges that have one vertex in C_r *and another in* C_s*, in the case* $V_1 \cap V_2 = \varnothing$*, or* ***twice*** *the number of edges that have both vertices in* C_r*, in the case* $C_r = C_s$*.*

As an example, for the triangle and the following equitable partition, we will have the symmetrized quotient as below.

$X =$  $X/\pi =$ 

As $S = \tilde{S}D$, for the diagonal $D_r = 1/\sqrt{|C_r|}$, we must have

$$\begin{aligned} C &= D\tilde{S}^* A \tilde{S} D \\ &= D\tilde{S}^* \tilde{S} B D \\ &= D\tilde{S}^* \tilde{S} D D^{-1} B D \\ &= S^* S D^{-1} B D \\ &= D^{-1} B D, \end{aligned}$$

from where C and B are conjugated by a positive diagonal. In fact, C is *the only* symmetric matrix conjugated to A by a positive diagonal.

We also have some information on the spectrum of C.

Proposition 6.5. *Let π be an equitable partition over X. Then*

$$\sigma(X/\pi) = \{\lambda \in \sigma(X) \colon \xi_\lambda \textit{ is constant on the cells of } \pi\},$$

where ξ_λ is an eigenvector related to the eigenvalue λ. Moreover, if $\lambda \in \sigma(X) \setminus \sigma(X/\pi)$ then for any eigenvalue ξ_λ we have

$$\sum_{r \in C_k} (\xi_\lambda)_r = 0 \qquad \forall k. \tag{$*$}$$

Proof. Suppose ξ is a λ-eigenvector of A. If $SS^*\xi =: \zeta \neq 0$, then

$$A\zeta = ASS^*\xi = SS^*A\xi = \lambda\zeta,$$

and thus ζ is also an eigenvector corresponding to λ. Moreover, $S^*\zeta$ is an eigenvector of C because

$$CS^*\zeta = S^*ASS^*\zeta = S^*SS^*A\zeta = \lambda S^*\zeta,$$

and as $SS^*\zeta = \zeta$, we have $S^*\zeta \neq 0$. Similarly, if ζ is an eigenvector of X/π corresponding to λ, then $S\zeta$ is an eigenvector of X corresponding to λ, and as $SS^*S\zeta = S\zeta$ we have $S\zeta \in \operatorname{col} SS^*$. Since SS^* projects onto the subspace of vectors that are constant on the cells of π, this completes the first part of the proposition.

For the second part, if $\lambda \in \sigma(X) \setminus \sigma(X/\pi)$, then for any eigenvector ξ related to λ, we must have $SS^*\xi = 0$, meaning that ξ is orthogonal to $\operatorname{col} S$. This is equivalent to $(*)$. □

The next lemma gives us information that links PST in X and X/π:

Lemma 6.6. *Let π be an equitable partition of X, which has a cell consisting of a singleton $\{a\} := \hat{a}$. Let C be the adjacency matrix of X/π and $\hat{b}$ the cell containing $b \in V(X)$. Then, for any time t:*

(1) $(e^{itA})e_a$ is constant in the cells of π;

(2) $(e^{itA})_{a,b} = (|\hat{b}|^{-\frac{1}{2}})(e^{itC})_{\hat{a},\hat{b}}$.

Proof. For (1), call S the normalized characteristic matrix of π. As $\{a\}$ is a cell, we have

$$e^{itA} e_a = e^{itA} S e_{\hat{a}}.$$

Since $\operatorname{col} S$ is A-invariant, it must also be e^{itA}-invariant, so any column of $e^{itA}S$ is constant in the cells of π. In particular, $e^{itA}e_a$ is constant in the cells of π.

Now, for (2), since $S^*S = I$ and SS^* commutes with A, we have

$$S^* e^{itA} S = e^{itS^*AS} = e^{itC},$$

which allows us to use (1) and the fact that the columns of e^{itA} sums to 1 to conclude (2). □

We can conclude from (2) of the previous lemma that:

Proposition 6.7. *Let X be a graph with an equitable partition π, such that the cells of a and b are singleton. Then, a and b have PST at time t iff $\hat{a}, \hat{b}$, in the symmetrized quotient graph, have PST at time t.*

6.2 Miscellaneous results

This section will present some original results concerning the symmetrized quotient graph. Our main motivation stems from the theory of fractional isomorphism, which is discussed in [25] and characterizes conditions for two graphs to have a non-symmetric quotient in common. We shall begin by defining:

Definition 6.8. *A non-negative matrix M is called* ***doubly stochastic*** *if $\mathbb{1}^*M = \mathbb{1}^*$ and $M\mathbb{1} = \mathbb{1}$.*

The following theorem is due to [25], and the last item due to [17]:

Theorem 6.9 (Ullman)**.** *For two graphs X, Y, it is equivalent:*

(1) There is a doubly-stochastic matrix M such that $A(X)M = MA(Y)$;

(2) X, Y have some common equitable partition;

(3) X, Y have in common the coarsest equitable partition;

(4) $D(X) = D(Y)$;

(5) $W_X = PW_Y$, for some permutation P.

The definition of *coarsest* will be seen later in this section, in Definition 6.12, while the definitions necessary to understand item (4) of the Theorem above are beyond the scope of this work. Nevertheless, it is worth mentioning that they are connected to the Weisfeiler-Lehman algorithm to decide graph isomorphism. We point out that we still do not have the analogous condition to this one for the upcoming Theorem 6.11.

Our main goal is to present similar conditions to the ones in the above theorem for two matrices having a common *symmetrized* quotient graph. We start with some definitions and lemmas arising from the fractional isomorphism theory, whose demonstration can be found in [25].

A matrix M is called decomposable if, for some permutation P, we have

$$PMP^* = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix},$$

where A, B are square matrices. If M is not decomposable, it is called indecomposable.

The proof of the following lemma can be found in [25].

Lemma 6.10. *If M is non-negative, doubly stochastic, and indecomposable, then M is irreducible.*

We present our novel theorem, which gives us a criterion for two matrices to have a common symmetrized quotient.

Theorem 6.11. *Let X and Y be graphs with adjacency matrices A and B. There are equitable partitions π_1 in X and π_2 in Y with equal symmetrized quotient graphs, that is $X/\pi_1 \cong Y/\pi_2$, iff there is a non-negative matrix M satisfying:*

(1) Both MM^* and M^*M are doubly stochastic.

(2) $AM = MB$.

Proof. Let R and S be normalized matrices related to equitable partitions of A and B, respectively, satisfying the equation

$$S^*AS = R^*BR.$$

We have

$$(SS^*)ASR^* = SR^*B(RR^*),$$

then

$$AS(S^*S)R^* = S(R^*R)R^*B,$$

hence

$$ASR^* = SR^*B.$$

The matrix SR^* is non-negative, as both R and S are non-negative. Furthermore, it satisfies (2), since

$$(SR^*)^*SR^* = R(S^*S)R^* = RR^*,$$

and

$$SR^*(SR^*)^* = S(R^*R)S^* = SS^*,$$

which are both doubly stochastic, as they are projectors onto the vectors that are constant on the partition classes, one of which is equal to $\mathbb{1}$.

Moving on to the converse, suppose a matrix M satisfying the theorem's conditions exists. In this case, MM^* commutes with A since

$$AMM^* = MBM^* = (MBM^*)^* = MM^*A.$$

From Lemma 6.10, we know that there exists some permutation P such that

$$MM^* = P \begin{pmatrix} S_1 & & & & \\ & S_2 & & & \\ & & S_3 & & \\ & & & \ddots & \\ & & & & S_k \end{pmatrix} P^*,$$

where S_r is irreducible. Let us denote

$$A = P \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1k} \\ A_{21} & A_{22} & \dots & A_{2k} \\ & & \ddots & \\ A_{k1} & A_{k2} & \dots & A_{kk} \end{pmatrix} P^*,$$

with the same block sizes as P^*MM^*P. The equation $AMM^* = MM^*A$ is equivalent to

$$S_rA_{rs} = A_{rs}S_s \qquad \forall r, s.$$

Multiplying by $\mathbb{1}$ we get

$$S_rA_{rs}\mathbb{1} = A_{rs}S_s\mathbb{1},$$

$$S_rA_{rs}\mathbb{1} = A_{rs}\mathbb{1},$$

and because S_r is irreducible, by Perron-Frobenius we have $A_{rs}\mathbb{1} = c\mathbb{1}$, which means that these blocks form an equitable partition on A.

In this partition, we will have that a and b are in the same cell iff they are in some irreducible block of MM^*, that is, $(MM^*)^k_{a,b} \neq 0$ for some k. Let us denote this cell of the equitable partition by C_r and denote by χ_r its characteristic vector, that is

$$(\chi_r)_a = \begin{cases} 1 & a \in C_r \\ 0 & a \notin C_r \end{cases}.$$

We will demonstrate that $M^*\chi_r$ corresponds in some way to a cell of an equitable partition in B.

We can use a similar argument to see that partitioning M^*M into classes of indecomposable blocks results in an equitable partition. Now, we aim to show that $M^*\chi_r$ is supported on one of these classes and is constant on its support.

To prove the first point, we will suppose that a and b are in the support of $M^*\chi_r$ and prove that $(M^*M)^k_{a,b} \neq 0$ for some k. The support is non-empty, for $MM^*\chi_r \neq 0$. Using the decomposition in blocks, each 1-eigenvector ζ satisfies

$$P \begin{pmatrix} S_1 & & & & \\ & S_2 & & & \\ & & S_3 & & \\ & & & \ddots & \\ & & & & S_k \end{pmatrix} P^*\zeta = \zeta,$$

from where each block of $P^*\zeta$ is an eigenvector of S_s. As S_s is indecomposable, by Perron-Frobenius, we must have that ζ is constant in these blocks. Hence, $\{\chi_s\}_s$ forms a basis for the 1-eigenspace of MM^* and the related eigenprojector is $\sum \alpha_s \chi_s \chi_s^*$, for $\alpha_s = \|\chi_s\|^{-2} > 0$. We have

$$\left(\sum M^*\alpha_s\chi_s\chi_s^*M\right)_{a,b} \geq \alpha_r \left(M^*\chi_r\chi_r^*M\right)_{a,b} = \alpha_r(M^*\chi_r)_a(M^*\chi_r)_b > 0.$$

Now, let $f = \sum c_s x^s$ such that $f(MM^*) = \sum \alpha_s\chi_s\chi_s^*$. Suppose by contradiction that a and b are not in the same indecomposable block of M^*M. This would imply that $((M^*M)^s)_{a,b} = 0$ for any $s > 0$, whence

$$\begin{aligned} 0 &= \left(\sum \alpha_s (M^*M)^{s+1}\right)_{a,b} \\ &= \left(M^*\left(\sum \alpha_r (MM^*)^s\right) M\right)_{a,b} \\ &= \left(M^*\left(\sum \alpha_s\chi_s\chi_s^*\right) M\right)_{a,b}, \end{aligned}$$

a contradiction. Hence, we can conclude that both a and b belong to the same cell within the equitable partition of B associated with M^*M. Let $C_{\sigma(r)}$ represent the cell that contains $\operatorname{supp} M^*\chi_r$, and let $\chi_{\sigma(r)}$ be its characteristic vector (we emphasize that this notation is for a whole new class of vectors, whose entries are in the vertices of B, and not just a permutation of the indices on χ_r). Considering the expression $(M^*M)(M^*\chi_r) = M^*(MM^*\chi_r) = M^*\chi_r$, we observe that $M^*\chi_r$ is an eigenvector of M^*M, just like $\chi_{\sigma(r)}$. If we examine the submatrix of M^*M with entries in $C_{\sigma(r)}$, we notice that the restriction of $M^*\chi_{\sigma(r)}$ to the entries of this submatrix remains an eigenvector within the submatrix. This is because $M^*\chi_{\sigma(r)}$ is supported on $C_{\sigma(r)}$. Furthermore, since this submatrix is irreducible, the Perron-Frobenius theorem states that only one eigenvector has positive entries (up to scalar multiplication). As $\mathbb{1}$ is also an eigenvector of this submatrix, we can conclude that $M^*\chi_r \parallel \chi_{\sigma(r)}$.

We will now demonstrate that the function $\sigma\colon r \mapsto \sigma(r)$ establishes an isomorphism between the respective quotient graphs. Since $\sum \chi_r = \mathbb{1}$ and $M^*\mathbb{1}$ are supported on all entries (if M^* has a row equal to zero, then M^*M would not be doubly-stochastic), and since M^* is non-negative, it follows that all cells of the equitable partitions are covered by $\{\chi_{\sigma(r)}\}_r$, or, in others words, σ is onto.

Also, σ is one-to-one, since:

$$\chi_{\sigma(r)} = \chi_{\sigma(s)} \implies M^*\chi_r \parallel M^*\chi_s \implies MM^*\chi_r \parallel MM^*\chi_s \implies r = s.$$

At last, we shall prove that it is an isomorphism. We begin by noting that

$$\|M^*\chi_r\|^2 = \chi_r^*(MM^*\chi_r) = \chi_r^*\chi_r,$$

from where

$$\frac{M^*\chi_r}{\sqrt{\chi_r^*\chi_r}} = \frac{\chi_{\sigma(r)}}{\sqrt{\chi_{\sigma(r)}^*\chi_{\sigma(r)}}}.$$

Thus, a direct calculation gives us

$$\begin{aligned}
\frac{\chi_{\sigma(r)}^*}{\sqrt{\chi_{\sigma(r)}^*\chi_{\sigma(r)}}} B \frac{\chi_{\sigma(s)}}{\sqrt{\chi_{\sigma(s)}^*\chi_{\sigma(s)}}} &= \frac{\chi_r^*}{\sqrt{\chi_r^*\chi_r}} MBM^* \frac{\chi_s}{\sqrt{\chi_s^*\chi_s}} \\
&= \frac{\chi_r^*}{\sqrt{\chi_r^*\chi_r}} AMM^* \frac{\chi_s}{\sqrt{\chi_s^*\chi_s}} \\
&= \frac{\chi_r^*}{\sqrt{\chi_r^*\chi_r}} A \frac{\chi_s}{\sqrt{\chi_s^*\chi_s}}
\end{aligned}$$

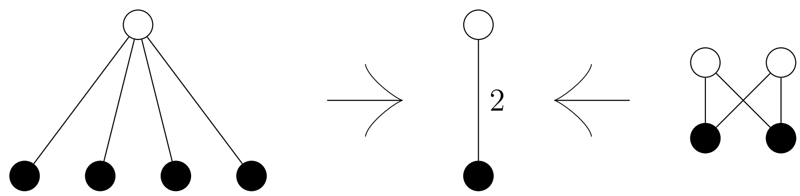
or, likewise

$$\frac{N(C_{\sigma(r)}, C_{\sigma(s)})}{\sqrt{|C_{\sigma(r)}||C_{\sigma(s)}|}} = \frac{N(C_r, C_s)}{\sqrt{|C_r||C_s|}},$$

which completes the proof that σ is an isomorphism. □

A crucial observation is that M is not necessarily a square matrix, as the graphs X and Y can have a different number of vertices and yet quotient into a common graph.

Such an example would be



whose related matrices are

$$\begin{pmatrix} & 1 & 1 & 1 & 1 \\ 1 & & & & \\ 1 & & & & \\ 1 & & & & \\ 1 & & & & \end{pmatrix} \frac{1}{2\sqrt{2}} \begin{pmatrix} 2 & 2 & & \\ & & 1 & 1 \\ & & 1 & 1 \\ & & 1 & 1 \\ & & 1 & 1 \end{pmatrix} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 2 & 2 & & \\ & & 1 & 1 \\ & & 1 & 1 \\ & & 1 & 1 \\ & & 1 & 1 \end{pmatrix} \begin{pmatrix} & & 1 & 1 \\ & & 1 & 1 \\ 1 & 1 & & \\ 1 & 1 & & \end{pmatrix}.$$

In general, it is easy to see that $K_{r,s}$ and $K_{r',s'}$ have a common symmetrized quotient if $rs = r's'$.

We may have different equitable partitions in the same graph. Some of them are comparable, using the relation:

Definition 6.12. *Let π, μ be two partitions of a graph. We say that μ is* ***coarser*** *than π, and denote by $\pi \leq \mu$, when each cell of π is contained in some cell of μ. In this case, we can also say that π is* ***finer*** *than μ.*

Given two partitions, π, μ, there is the finest partition coarser than both, which is said to be π ***join*** *μ and is denoted by $\pi \vee \mu$. This partition can be defined by:*

$$a \sim_{\pi \vee \mu} b \iff \exists x_1, \dots, x_r; a \sim_\pi x_1 \sim_\mu x_2 \cdots \sim_\pi x_r \sim_\mu b,$$

where $a \sim_\nu b$ means $\nu(a) = \nu(b)$ for a partition ν.

These definitions are for general partitions, not necessarily equitable ones. The first result relating them to equitable partitions is the following proposition, from [25]:

Proposition 6.13. *Suppose π, μ are equitable partitions of X. Then so is $\pi \vee \mu$.*

Moreover, all graphs have a finest equitable partition, the trivial one (each cell is a singleton). Also, joining all equitable partitions will give us the coarsest equitable partition, which is unique. We can also prove that the equitable partitions of a graph forms a lattice [25].

Definition 6.14. *A* ***lattice*** *is a poset in which each pair of elements has a join and a meet, (i.e., a supremum and an infimum).*

From now on, we shall denote this poset by $\mathcal{E}(X)$. We need the following lemma, whose proof can be found in [2].

Lemma 6.15. *An orthogonal projector P has non-negative entries iff $\operatorname{rng} P$ has a non-negative orthonormal basis.*

With that, we can relate projectors and equitable partitions by our novel theorem:

Theorem 6.16. *Let X be a graph. The following function is a bijection*

$$\varphi\colon \mathcal{E}(X) \to \mathcal{P}(X)$$

$$\pi \mapsto P_\pi := S(\pi)S(\pi)^*,$$

where $\mathcal{P}(X)$ is the set of all non-negative orthogonal projectors that commutes with $A(X)$ and has $\mathbb{1}$ in its range.

Moreover,

(1)

$$\pi \leq \mu \iff P_\pi \geq P_\mu \iff \operatorname{rng} P_\pi \supseteq \operatorname{rng} P_\mu,$$

(2)

$$P_{\pi\vee\mu} = P_{\operatorname{rng} P_\pi \cap \operatorname{rng} P_\mu},$$

(3)

$$A(X/\pi) = A(X)|\operatorname{rng} P_\pi,$$

where we use as basis for $\operatorname{rng} P_\pi$ the columns of S_π. Here, $A(X/\pi) = A(X)|\operatorname{rng} P_\pi$ means the restriction of the linear transformation induced by multiplying by A to the subspace $\operatorname{rng} P_\pi$.

Proof. The range of φ is indeed in $\mathcal{P}(X)$. To see that φ is one-to-one, let $\pi \neq \mu$ be two equitable partitions of X. As they are different, we have some pair a, b for which $\pi(a) = \pi(b)$ and $\mu(a) \neq \mu(b)$ (or vice versa, but the other case is similar). This implies that $(P_\mu)_{a,b} = 0 \neq (P_\pi)_{a,b}$. Here we recall that it follows from the definition and a simple calculation that

$$(P_\pi)_{a,b} = \begin{cases} \frac{1}{|C_{\pi(a)}|}, & \pi(a) = \pi(b) \\ 0, & \pi(a) \neq \pi(b). \end{cases}$$

Now, let $P \in \mathcal{P}(X)$ be arbitrary. Using Lemma 6.15, we have an orthonormal basis ζ_r of non-negative vectors for $\operatorname{rng} P$. As ζ_r are non-negative, we must have for $r \neq s$ that $\operatorname{supp} \zeta_r \cap \operatorname{supp} \zeta_s = \varnothing$ to ensure orthogonality. Also, each ζ_r must be constant in its support since summing another ζ_s cannot alter the values in $\operatorname{supp} \zeta_r$, and there is some linear combination of them which results in $\mathbb{1}$. Hence, we conclude that $P = S_\pi$, where π is the partition into $\{\operatorname{supp} \zeta_r\}_r$. It must be an equitable partition, for it commutes with A.

(1) follows from the fact that $\pi \leq \mu$ iff $\operatorname{col} S(\pi) \supseteq \operatorname{col} S(\mu)$, combined with the property $\operatorname{rng} P_\pi = \operatorname{col} S(\pi)$.

Based on (1), we can conclude that $\operatorname{rng} P_{\pi\vee\mu}$ is the largest vector space which is contained in both $\operatorname{rng} P_\pi$ and $\operatorname{rng} P_\mu$, and whose projector is also in $\mathcal{P}(X)$. The projector onto $\operatorname{rng} P_\pi \cap \operatorname{rng} P_\mu$ is indeed in $\mathcal{P}(X)$ since it is the limit of non-negative operators that commute with A: let $P = \lim_n (P_\pi P_\mu P_\pi)^n$. P indeed exists and is a projector: all entries of the Jordan matrix of $P_\pi P_\mu P_\pi$ converge to zero, except the ones in the diagonal. It is self-adjoint as it is the limit of self-adjoint operators, and $\operatorname{rng} P = \operatorname{rng} P_\pi \cap \operatorname{rng} P_\mu$ because as $P_\pi P_\mu P_\pi$ is a contraction, the fix points of the convergent are the same as the fixed points of $P_\pi P_\mu P_\pi$, which are $\operatorname{rng} P_\pi \cap \operatorname{rng} P_\mu$.

For (3), suppose S is $m \times n$. $S\colon \mathbb{R}^n \to P_\pi$ is an isomorphism, since $\langle Sv, Sw\rangle = v^* S^* S w = v^* w$ and $\operatorname{col} S = \operatorname{rng} P_\pi$. Furthermore, the following diagram commutes

$$\begin{array}{ccc} \operatorname{rng} P_\pi & \xrightarrow{A|\operatorname{rng} P_\pi} & \operatorname{rng} P_\pi \\ \downarrow{\scriptstyle S^*} & & \downarrow{\scriptstyle S^*} \\ \mathbb{R}^n & \xrightarrow{S^*AS} & \mathbb{R}^n \end{array},$$

which concludes what we wanted. In $\operatorname{rng} P_\pi$, we must use the basis $\operatorname{col} S$, obtained as the image of the canonical basis in $\mathbb{R}^n$, to have equality in the matrices related to the linear transformations.

□

For our following proof, we will return to the non-normalized quotient of graphs. The quotients in the following theorem refer to the non-symmetrized digraph. This original result demonstrates that its non-symmetrized quotient inherits the equitable partitions of the initial graph.

Theorem 6.17. *Let X be a graph on n vertices. Let $\mu \in \mathcal{E}(X)$. Denote by $S(\pi)$ the non-normalized characteristic matrix of a partition π, in particular $R := S(\mu)$, and let D be the diagonal matrix with $D_r = 1/|\mu^{-1}(r)|$. Define the function*

$$\varphi\colon \{\pi \in \mathcal{E}(X)\colon \mu \le \pi\} \to \mathcal{E}(X/\mu),$$

$$\pi \mapsto DR^* S(\pi)$$

$$RM \hookleftarrow M,$$

where we are identifying a partition with its characteristic matrix. Then φ is an order-preserving bijection, and we also have

$$(X/\mu)/\varphi(\pi) \cong X/\pi.$$

Proof. Fix some $\pi \in \mathcal{E}(X)$ and denote $S := S(\pi)$. A direct calculation gives us that

$$(R^*S)_{r,s} = \sum_a R_{a,r} S_{a,s} = \begin{cases} 0 & \mu^{-1}(r) \not\subseteq \pi^{-1}(s) \\ |\mu^{-1}(r)| & \mu^{-1}(r) \subseteq \pi^{-1}(s) \end{cases}$$

From where we see that DR^*S is the matrix related to the partition induced by S on the classes of R. Another calculation gives us that

$$DR^*R = R^*RD = I,$$

from where RDR^* is a projector onto the vectors constant on the classes of μ. Calling B the adjacency matrix of X/μ and C the adjacency matrix of X/π we know that

$$AR = RB, \qquad AS = SC,$$

from where we want to show that

$$B(DR^*S) = (DR^*S)C,$$

which proves that DR^*S is the characteristic matrix of an equitable partition of B and the compatibility of the quotients.

As $\mu \leq \pi$, the columns of S are on the range of RDR^*, hence

$$RDR^*S = S,$$

and thus

$$\begin{aligned} B(DR^*S) &= (I)BDS^*R \\ &= (DR^*R)BDS^*R \\ &= DR^*(RB)DS^*R \\ &= DR^*(AR)DR^*S \\ &= DR^*A(RDR^*S) \\ &= DR^*A(S) \\ &= DR^*(AS) \\ &= DR^*(SC), \end{aligned}$$

concluding the first part of the proof. To see that φ is one-to-one, a simple calculation gives us

$$DR^*S(\pi) = DR^*S(\nu) \implies RDR^*S(\pi) = RDR^*S(\nu) \implies S(\pi) = S(\nu).$$

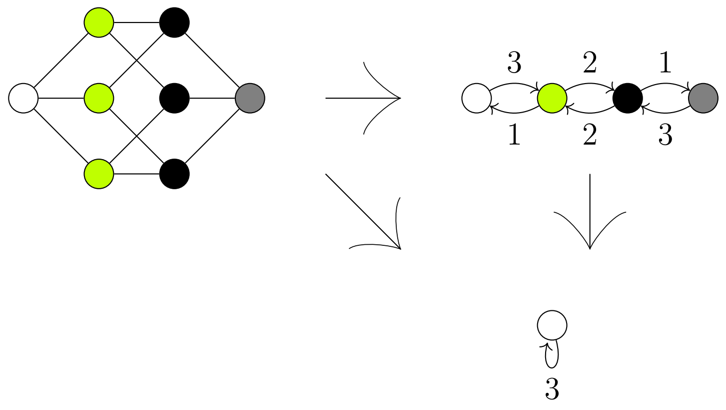
For each M that is a non-normalized matrix of an equitable partition of B, we have $BM = MC$ for some C. Applying R we get

$$(RB)M = RMC \implies ARM = RMC.$$

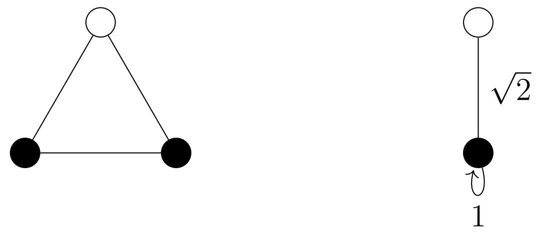
As each line of R has only one non-zero entry, we can also conclude that RM is a matrix of 0's and 1's. Thus, it is an equitable partition of A. As $DR^*RM = M$, the image of RM is indeed M, as we wanted.

We note that $\pi \leq \nu$ iff $\operatorname{rng} S(\pi) \supseteq \operatorname{rng} S(\nu)$, and as the composition of functions preserves the inclusion of their range, we conclude that φ preserves order. □

As an example of how the equitable partitions are inherited by the quotient graphs, we can present the cube $P_2^{\square 3}$:



It would be desirable if Theorem 6.17 was true for the symmetrized quotient and equitable partitions. However, it is not the case, as we can see in this simple example:



In C_3, we have two equitable partitions: the one with a white cell and a black cell and the coarser equitable partition, which possesses only one cell. However, when we quotient the graph by the first partition, the quotient graph does not possess any non-trivial equitable partition.

However, there is a particular case when the symmetrized equitable partitions do pass to the quotient:

Proposition 6.18. *Let $\mu \leq \pi$ be equitable partitions of X, and denote P, S their respective normalized partition matrices. Suppose that for each cell C of π, each cell of μ contained in C has the same size. Then, the partition of X/μ into the cells induced by π is equitable. Denoting it by ν, we have $(X/\mu)/\nu \cong X/\pi$. Moreover, the normalized partition matrix of ν is P^*S.*

Proof. We note that $\mu \leq \pi$ iff $PP^*SS^* = SS^*PP^* = SS^*$. The matrix P^*S has indeed orthonormal columns, for

$$\begin{aligned}
(P^*S)_{rs} &= \sum_a P_{a,r}S_{a,s} \\
&= \frac{|C_r \cap \tilde{C}_s|}{\sqrt{|C_r|}\sqrt{|\tilde{C}_s|}} \\
&= \begin{cases} 0, & C_r \cap \tilde{C}_s = \varnothing \\ \frac{1}{\sqrt{|\tilde{C}_s|/|C_r|}}, & C_r \subseteq \tilde{C}_s \end{cases}.
\end{aligned}$$

As $\bigcup_{C_r \subseteq \tilde{C}_s} C_r = \tilde{C}_s$, each column has norm one. It is also constant because, by hypothesis, $|C_r|$ is constant within $\tilde{C}_s$. Two columns are also orthogonal since C_r is contained in only one cell of μ. Each characteristic vector of a class of π is constant in the cells of μ. Thus, each column of S must be PP^*-invariant, whence $PP^*S = S$ and

$$(P^*S)^*P^*AP(P^*S) = S^*AS;$$

as we wanted. Moreover

$$\begin{aligned}
P^*A(PP^*S)S^*P &= P^*A(S)S^*P \\
&= P^*A(SS^*)P \\
&= P^*(SS^*)AP \\
&= P^*S(S^*)AP \\
&= P^*S(S^*PP^*)AP.
\end{aligned}$$

That is, P^*SS^*P commutes with P^*AP; hence, it is an equitable partition. □

6.3 Constructing graphs with equitable partition

The following result and notations are inspired by [21].

We start this section by introducing a concept that will help reconstruct graphs from their quotient graph.

Definition 6.19. *Let Q be a weighted digraph without loops and with natural-valued edges. We say that $w\colon V(Q) \to \mathbb{N}$ is a **weight-function** if for each pair of vertices (r, s) and associated arc $e_{r,s}$ it satisfies*

(i) $w(r)e_{r,s} = w(s)e_{s,r}$,

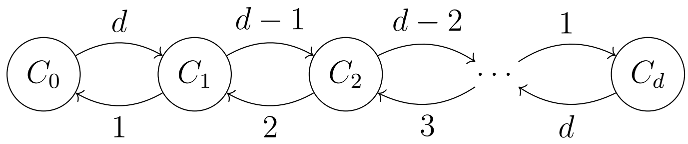
(ii) $w(s) \geq e_{r,s}$

This definition comes from when $Q = \widetilde{X/\pi}$, and $w(r) = |C_r|$. In this situation, it is clear that conditions $(i), (ii)$ are satisfied. Hence, if $Q \cong \widetilde{X/\pi}$ for some X and π, there is a weight function for Q.

As an example of a weight function, we can use the d-cube $P_2^{\square d}$. It is possible to partition the vertices of the cube into the classes

$$C_r := \{a \colon d(a, O) = r\}, \quad O := (0, 0, \ldots, 0).$$

We have $d(a, O) = r$ iff there are exactly r entries in a of value 1. Hence $|C_r| = \binom{d}{r}$. A vertex $a \in C_r$ has exactly $d - r$ neighbors in C_{r+1}, which are obtained by changing an entry with value 0 to the value 1. Similarly, a vertex in C_r has r neighbors in C_{r-1}, this time obtained by changing a 1 to a 0. Hence, $\{C_r\}$ defines indeed an equitable partition, and its quotient is naturally represented by the following digraph:



The related weight-function is $w(C_r) = \binom{d}{r}$.

The conditions on Definition 6.19 are also sufficient for Q being of the form $Q \cong \widetilde{X/\pi}$.

Proposition 6.20. *Given a graph Q with a weight-function w we can construct a graph X which posses an equitable partition $\pi \colon V(X) \to V(Q)$ such that $|C_r| = w(r)$ and $\widetilde{X/\pi} \cong Q$.*

Proof. We can explicitly construct X. Let $C_r = \{0, \ldots, w(r) - 1\} \times \{r\}$ and for $r < s$ we define

$$(a, r) \sim (b, s) \iff \exists k,\ ae_{r,s} \leq k < (a+1)e_{r,s};\ a + k \equiv b \mod w(s).$$

Condition (ii) ensures that each vertex in C_r has exactly $e_{r,s}$ neighbors in C_s since each k in the above equation will correspond to a different vertex.

The edges from C_r to C_s form the set

$$\{(0,0), (0,1), \ldots, (0, e_{r,s} - 1), (1, e_{r,s}), \ldots, (w(r) - 1, w(r)e_{r,s} - 1)\}.$$

(Here, we omit the second coordinate r and s of the vertices and the second coordinate is being taken modulo $w(s)$).

As $w(s) \mid w(r)e_{r,s}$ this set covers each vertex of C_s exactly $w(r)/w(s)e_{r,s} = e_{s,r}$ times; or, in others words, each vertex in C_s has $e_{s,r}$ neighbors in C_r. □

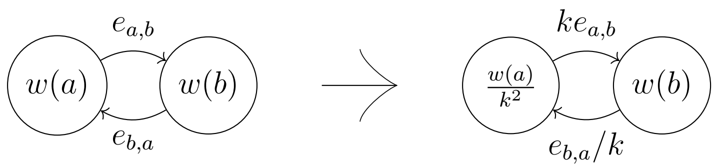
Consider a weighted directed graph Q. We define the weighted graph $\check{Q}$ as the **symmetrization** of Q, where $V(\check{Q}) = V(Q)$ and the weight of the edge ab in $\check{Q}$ is equal to the geometric mean of the arcs ab and ba in Q. It is worth noting that if $\widetilde{X/\pi} \cong Q$, then $X/\pi \cong \check{Q}$. This observation, along with Proposition 6.7, yields the following result:

Proposition 6.21. *Suppose Q is digraph with weight-function w such that $\check{Q}$ exhibits PST between vertices a and b, and $w(a) = w(b) = 1$. Then, the graph obtained by Proposition 6.20 also possesses PST between the vertices associated with a and b. Moreover, the number of vertices in the new graph is equal to the sum of the weights of the vertices in Q.*

This construction allows us to work with a given graph Q with weight function w, which we know to have PST between vertices a, b with $w(a) = w(b) = 1$, and change the values of its arcs and weight function without changing $\check{Q}$. This property leads to a simplification rule:

Given a graph Q with weight function w, if we have for some pair of vertices a, b an integer k such that $k^2 \mid w(a)$, $k \mid e_{b,a}$ and $2e_{a,b} \leq w(b)$ then we can make the following substitution maintaining properties $(i), (ii)$ and reducing the total weight of the graph:

$$\begin{cases} w(a) \hookleftarrow \frac{w(a)}{k^2} \\ e_{a,b} \hookleftarrow ke_{a,b} \\ e_{b,a} \hookleftarrow e_{b,a}/2 \end{cases}$$



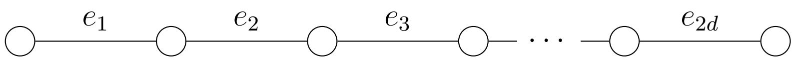
In the d-cube, these conditions translate to finding values for r and k such that

$$\begin{cases} k^2 \mid \binom{d}{r} \\ k \mid r+1 \\ 2(d-r) \leq \binom{d}{r+1} \end{cases}$$

More rules like this one can be found on [21], which we will not include here since it would drift too far from the objective of focusing in PST on weighted paths.

6.4 Un-quotienting weighted paths

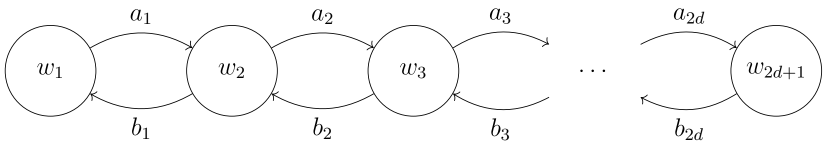
This section will show how to apply Proposition 6.21 when the graph is a weighted path. Suppose that X is a weighted non-directed path with PST between extremities. We will also assume that X has no loops, which is equivalent to assuming that $a_r = 0$ on the related tridiagonal matrix. This will occur iff the eigenvalues of X are symmetric concerning the origin, and for that, we will also need the number of vertices on the graph to be odd, let us say $2d+1$ (or the spectrum to be semi-integers, but we are avoiding this case). Then, X will be of the form



and will be uniquely defined by the sequence

$$e_1, e_2, \dots, e_{2d}.$$

All the possible values for e_r can be retrieved algorithmically using Theorem 5.14. Now, we want to obtain X a graph whose symmetrization is X, together with a weight function w:



where

(1) $a_r \leq w_{r+1}$;

(2) $b_r \leq w_r$;

(3) $w_r a_r = b_r w_{r+1}$;

(4) $a_r b_r = e_r^2$;

(5) $w_1 = w_{2d+1} = 1$;

(6) $a_r, b_r, w_r \in \mathbb{Z}$.

Conditions $(1) - (3)$ are the weight conditions, (4) tells us that the symmetrization of the digraph will result in its symmetrized version, and (5) tell us that the cells corresponding to the extremities are indeed singletons.

Condition (3) give us that

$$w_{r+1} = \frac{a_r}{b_r} w_r,$$

which allows us to conclude by induction and using (5) that

$$w_{r+1} = \frac{a_r a_{r-1} \cdots a_1}{b_r b_{r-1} \cdots b_1}.$$

We observe that given compatible values of a_r and b_r, we can obtain new compatible values $\tilde{a}_r$ and $\tilde{b}_r$ by taking:

For $\tilde{a}_r$:

$$a_1, \dots, a_d, b_d, b_{d-1}, \dots b_1;$$

For $\tilde{b}_r$:

$$b_1, \ldots, b_d, a_d, \ldots, a_1.$$

These new values for $\tilde{a}_r, \tilde{b}_r$ and $\tilde{w}_r := \dfrac{\tilde{a}_1 \cdots \tilde{a}_r}{\tilde{b}_1 \cdots \tilde{b}_r}$ satisfy (1) $\sim$ (6), by use of Theorem 5.13. Furthermore, the weight of $\tilde{a}_r$ and $\tilde{b}_r$ equals the original weight in the first half, and the weight in the second half equals the weight in the first half. Therefore, we can assume that the total weight of $\tilde{a}_r$ and $\tilde{b}_r$ is less than or equal to the initial weight (if the weight in the second half of a_r and b_r is smaller than in the first half, we can perform a similar reflected construction).

This argument allows us to assume that $a_{d+r-1} = a_r$ and $b_{d+r-1} = b_d$, which lowers the number of elements we want to compute. Also, the values of a_r can be determined by b_r since $a_r = e_r^2/b_r$.

We can resume the problem:

Problem 6.1. *Given the integer values* $e_1^2, \ldots, e_d^2$*, determine the sequence* $b_1, \ldots, b_d \in \mathbb{N}$ *which satisfies*

(1) $b_1 = 1$*;*
(2) $e_1^2 \cdots e_r^2 \geq b_1^2 \cdots b_r^2 b_{r+1}, \qquad r = 1, \ldots, d-1;$
(3) $b_r | e_r^2, \qquad r = 1, \ldots, d;$
(4) $b_1^2 \cdots b_r^2 | e_1^2 \cdots e_r^2 \qquad r = 1, \ldots, d;$

and minimize:

$$W = \frac{e_1^2 \cdots e_d^2}{b_1^2 \ldots b_d^2} + 2\left(\sum_{r=1}^{d-1} \frac{e_1^2 \cdots e_r^2}{b_1^2 \cdots b_r^2} + 1\right).$$

For instance, in the $(2d)$-cube, we have the values $e_r^2 = (2d-r+1)r$, and the values $b_r = r$ satisfies (1) $-$ (4) of the above problem. For small values of d, they are not the solution for Problem 6.1; however, it is still unknown whether the solution's total weight W also grows exponentially, as is the case of the total weight grows with these values of b_r.

Chapter 7

Conclusions

The main goal of the thesis was to work on the problem of Section 4.3, namely to obtain bounds (or the exact value) for $\mathfrak{N}$. From the literature, we already know how to find all weighted paths with PST between extremities, and given some weighted graphs, there are known combinatorial ways to get a related simple graph. Our objective was to delve deeper into these phenomena, which was done in the last two chapters.

In Chapter 5, we obtained a new way for obtaining weighted graphs with strongly cospectral vertices, with Theorem 5.18. However, to apply it to construct a PST, as in Theorem 5.21, we must first solve the algebraic Problem 5.1. This problem shows to be quite hard to approach, and we do not expect to have a general answer for it any soon. For instance, solving it for $d = 2k + 1$ would answer the Prouhet-Tarry-Escott problem, an open problem in number theory that has been researched since the 1700s. For the definition and results of this problem, see [6].

Despite Proposition 5.16 being enough to calculate orthogonal polynomials for the case of PST between an extremity and another vertex, this formula cannot be used to directly construct polynomials which determine paths with PST between two arbitrary vertices: in this case, the spectral support of the vertex can be different from the spectrum, and this would imply that its related polynomial has some zero in common with the P_{d+1}, case which Proposition 5.16 does not cover. We have approached this question algebraically using the Christoffel-Darboux theorem and obtained a general formula; however, the generalization of the following propositions and corollaries is incomplete. We are currently doing more profound research into these problems.

Chapter 6 was the link between the main problem and Chapter 5. In this chapter, we obtained new results involving quotient graphs, including Theorem 6.11, which is a generalization of a significant result with applications in the perfect state transfer theory, besides the general theory of algebraic combinatorics. In the last two sections, we approached the problem more directly and obtained conditions for constructing a simple graph together with its weight (number of vertices).

Section 6.4 gives us a condition for having some graph that can be quotiented into a given weighted path. These conditions are general, and they determine all graphs with these properties. We have implemented Theorem 5.14 in Python and computed the values of e_r^2 for a wide range of spectra. Moreover, we have made a greedy algorithm to estimate the values of W in Problem 6.1. However, this approach has been proved inefficient, and we could at most obtain the bound $\mathfrak{N} \leq 0.847$.

For better approximations of $\mathfrak{N}$, we need a better optimization for solving Problem 6.1. The best bound for $\mathfrak{N}$ was obtained using *pseudo-equitable* partition in hyper-cubes, $P_2^{\square n}$. Using pseudo-equitable partitions is another excellent option to explore for better results, as has been done in [10, 21].

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