Graph Spectra and Continuous Quantum Walks

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Preface

If A is the adjacency matrix of a graph X, we define a transition matrix $U(t)$ by

$$U(t) = \exp(\mathrm{i}tA).$$

Physicists say that $U(t)$ determines a *continuous quantum walk*. Most questions they ask about these matrices concern the squared absolute values of the entries of $U(t)$ (because these may be determined by measurement, and the entries themselves cannot be). The matrices $U(t)$ are unitary and $\overline{U(t)} = U(-t)$, so we may say that the physicists are concerned with questions about the entries of the Schur product

$$M(t) = U(t) \circ \overline{U(t)} = U(t) \circ U(-t).$$

Since $U(t)$ is unitary, the matrix $M(t)$ is doubly stochastic. Hence each column determines a probability density on $V(X)$ and there are two extreme cases:

(a) A row of $M(t)$ has one nonzero entry (necessarily equal to 1).

(b) All entries in a row of $U(t)$ are equal to $1/|V(X)|$.

In case (a), there are vertices a and b of X such that $|U(t)_{a,b}| = 1$. If $a \neq b$, we have *perfect state transfer* from a to b at time t, otherwise we say that X is *periodic* at a at time t. Physicists are particularly interested in perfect state transfer. In case (b), if the entries of the a-row of $M(t)$ is constant, we have *local uniform mixing* at a at time t. (Somewhat surprisingly these two concepts are connected—in a number of cases, perfect state transfer and local uniform mixing occur on the same graph.)

The quest for graphs admitting perfect state transfer or uniform mixing has unveiled new results in spectral graph theory, and rich connections to other fields of mathematics. This also brought us to explore more topics in quantum information and their interplay with combinatorics. This book is, in part, a progress report on these questions.

For us, the biggest surprise is the extent to which tools from algebraic graph theory prove useful. So we treat this in somewhat more detail than is strictly necessary. Some of it is standard, some is old stuff repackaged, and some is new material (e.g., controllability, strongly cospectral vertices) that has been developed to deal with quantum walks. But combinatorics is not everything: we also meet with Lie groups, various flavours of number theory, and almost periodic functions. (And so a second surprise is the number of different mathematical areas entangled with our topic.)

We do not treat discrete quantum walks here (see [**?**]). We do not treat quantum algorithms or quantum computation, nor do we deal with questions about complexity, error correction, non-local games, and the quantum circuit model. We discuss a little of the related physics. We have focussed on questions that are both mathematically interesting and have some physical significance, since this overlap is often a sign of a fruitful outcome.

We have had useful comments on these notes from many people, including Dave Witte Morris, Tino Tamon, Sasha Jurišic and members of his seminar, Alexis Hunt, David Feder, Henry Liu, Harmony Zhan, Nicholas Lai, Xiaohong Zhang, Soffia Arnadottir, Qiuting Chen. . . .

This is a (VERY) preliminary version intended to be used a class notes for a grad course at UFMG in 2020. We welcome any comments to gabriel@dcc.ufmg.br or cgodsil@uwaterloo.ca.

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Part I

Introduction

Chapter 1

Continuous Quantum Walks

This chapter provides an overview of continuous-time quantum walks on graphs, from the viewpoint of a mathematician, with a strong focus on examples. We will discuss the underlying physics in the next chapter.

In the course of their work on quantum computing, physicists have introduced *continuous quantum walks*. To define such a walk, we take a real symmetric matrix H and define transition operators $U(t) = U_H(t)$ for $t \in \mathbb{R}$ by

$$U(t) := \exp(\mathrm{i}tH).$$

The matrix H is the *Hamiltonian* of the walk. Our default assumption is that H is the adjacency matrix of a graph, though most of our considerations apply to other models as well. We observe that $\overline{U(t)} = U(-t)$ and (since H is symmetric) that $U(t)^T = U(t)$. Hence

$$U(t)^* U(t) = U(-t)U(t) = I,$$

equivalently $U(t)$ is a unitary matrix for all t. (For a complex matrix U, we are using U^* to denote the conjugate-transpose $\overline{U}^T$ of U.)

We are in fact borrowing the terminology and the picture from the classical counterpart. A continuous random walk on a graph X can be specified by a family of matrices $M(t)$, where $M(t)_{a,b}$ is the probability that at time t the "walker" is on vertex b, given that it started at vertex a. In the classical case, we assume the underlying model is that in a short time interval of length δt, the walker moves to an adjacent vertex with probability proportional to δt, and it is equally likely to move to any neighbor of the vertex it is on. If A is the adjacency matrix of X and Δ is the diagonal matrix such that $\Delta_{a,a}$ is the valency of a, then standard theory for Markov chains in continuous time imply that

$$M(t) = \exp(t(A - \Delta)).$$

We note that each column of $M(t)$ is a probability density—its entries are nonnegative and sum to 1. There are some analogies to the quantum case, but in general the walks are very different.

Thoughout this book, the term “graph” means “finite graph”.

1.1 Basics

By way of example, take $X = P_2$ and $A = A(P_2)$.

Figure 1.1: The graph P_2.

Then

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and so, for any $k \in \mathbb{Z}$,

$$A^{2k} = I, \quad A^{2k+1} = A.$$

Therefore

$$\begin{aligned} \exp(\mathrm{i}tA) &= I + \mathrm{i}tA - \frac{1}{2}t^2 I - \frac{1}{6}\mathrm{i}t^3 A + \frac{1}{24}t^4 I + \cdots \\ &= \cos(t)I + \mathrm{i}\sin(t)A \end{aligned}$$

and

$$U(t) = \begin{pmatrix} \cos(t) & \mathrm{i}\sin(t) \\ \mathrm{i}\sin(t) & \cos(t) \end{pmatrix}.$$

At particular times t, this matrix takes a special form. For instance

$$U(\pi) = -I,$$

while

$$U(\pi/2) = \mathrm{i}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and

$$U(\pi/4) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}.$$

Thus $U(t)$ is respectively:

(a) A scalar matrix.

(b) A scalar times a permutation matrix.

(c) A unitary matrix with all entries having the same absolute value.

Given a graph X and a time t, we can define the mixing matrix $M(t)$ as the Schur or entry-wise product of $U(t)$ and its conjugate, that is,

$$M(t) = U(t) \circ U(-t).$$

For $a, b \in V(X)$, the entry $M(t)_{a,b}$ is the probability that at time t the quantum walk that started at a will terminate at b. In Chapter 2, we will elucidate what we mean by this in terms of quantum physics. For the path on two vertices we have

$$M(t) = \begin{pmatrix} \cos^2(t) & \sin^2(t) \\ \sin^2(t) & \cos^2(t) \end{pmatrix}.$$

Clearly the mixing matrix is (always) doubly stochastic, equivalently each row and column is a probability density. We will be most interested in determining if there is a time t such that a column of $M(t)$ takes a specified form: for example, whether some entry is equal to 1 (in which case all other entries are 0), or whether all entries are equal.

1.2 Products

The *Kronecker product* $A \otimes B$ of matrix A and B is the matrix we get if, for each i and j we replace the ij-entry of A by $A_{i,j}B$. So if A is $k \times \ell$ and B is $m \times n$, the product $A \otimes B$ is a matrix of order $km \times \ell n$.

The crucial property of the Kronecker product is that, if the products AC and BD are defined, then

$$(A \otimes B)(C \otimes D) = AC \otimes BD.$$

For example, $A \otimes B = (A \otimes I)(I \otimes B)$.

The Kronecker product provides a convenient way to define products of graphs. In particular if X and Y are graphs, their *Cartesian product* $X \square Y$ is defined as the graph on vertex set $V(G) \times V(H)$, where $(x, y) \sim (x', y')$ if $x = x'$ and $y \sim y'$ in Y or $x \sim x'$ in X and $y = y'$. If X and Y have respective adjacency matrices $A(X)$ and $A(Y)$, the adjacency matrix of their Cartesian product is

$$A(X \square Y) = A(X) \otimes I + I \otimes A(Y).$$

1.2.1 Lemma. *If X and Y are graphs, then, for any t,*

$$U_{X \square Y}(t) = U_X(t) \otimes U_Y(t).$$

Proof. Assume the adjacency matrices of X and Y are A and B respectively. The matrices $A \otimes I$ and $I \otimes B$ commute, whence

$$\begin{aligned} \exp(\mathrm{i}t(A \otimes I + I \otimes B)) &= \exp(\mathrm{i}t(A \otimes I)) \exp(\mathrm{i}t(I \otimes B)) \\ &= (\exp(\mathrm{i}tA) \otimes I)(I \otimes \exp(\mathrm{i}tB)) \\ &= \exp(\mathrm{i}tA) \otimes \exp(\mathrm{i}tB). \end{aligned}$$

□

It follows, for example, that the transition matrix for the d-cube $Q_d = P_2^{\square d}$ is the d-th tensor power of the transition matrix for P_2.

$$U_{Q_d} = U_{P_2}(t)^{\otimes d}.$$

If $L(X)$ denotes the Laplacian of X then you are invited to verify that

$$L(X \square Y) = (L(X) \otimes I) + (I \otimes L(Y)).$$

Hence whether we use the adjacency matrix or the Laplacian, the above lemma holds.

The Kronecker product interacts nicely with Schur product, thus if A and C have the same order and B and D have the same order,

$$(A \otimes B) \circ (C \otimes D) = (A \circ C) \otimes (B \circ D).$$

From this it follows that

$$M_{X \square Y}(t) = M_X(t) \otimes M_Y(t).$$

1.3 State Transfer and Mixing

Suppose A is a symmetric matrix, which we view as a weighted adjacency matrix of a graph X. (Hence it could be an adjacency matrix, a signed adjacency matrix, or a Laplacian.) If $a \in V(X)$, we denote its characteristic vector by e_a, that is, the vector in $\mathbb{R}^{V(X)}$ that is 0 in all entries except for the entry corresponding to a, which is equal to 1.

We say that we have *perfect state transfer* from vertex a in X to vertex b at time t if

$$M(t)_{a,b} = 1.$$

Since $U(t)$ is unitary, this is equivalent to having a complex scalar γ of absolute value equal to 1 such that

$$U(t)e_a = \gamma e_b.$$

This complex number γ is called the *phase factor*. In Chapter 2 we will discuss the (ir)relevance of γ. From Section 1.1 we see that if $A = A(P_2)$, we have perfect state transfer from vertex a to vertex b at time $\pi/2$. From Section 1.2 it follows that if a is a vertex in the d-cube $Q_d = P_2^{\square d}$, then at time $\pi/2$ we have perfect state transfer from a to the unique vertex at distance d from a.

We say that we have *instantaneous uniform mixing*, or just *uniform mixing* at time t if all entries of $M(t)$ are equal, or, equivalently, if all entries of $U(t)$ have the same absolute value. (We say that a matrix with this property is *flat*.) For P_2 we saw that $U(\pi/4)$ is flat. Hence we have uniform mixing at time $\pi/4$ on P_2 and, more generally, on the d-cube Q_d.

Two of our basic problems are to determine the cases where perfect state transfer occurs, and to determine the cases where uniform mixing occurs.

1.4 Symmetry and Periodicity

We saw that at time $\pi/2$ we have perfect state transfer on P_2 from vertex a to vertex b and, at the same time, from vertex b to vertex a. Similarly, on P_3,

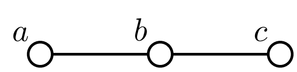

Figure 1.2: The graph P_3.

we will see in Section 1.6 that we have perfect state transfer for a to c, and from c to a, at time $\pi/\sqrt{2}$. These are examples of something much more general.

1.4.1 Lemma. *If we have perfect state transfer on X from vertex a to vertex b at time τ, then we have perfect state transfer from b to a at the same time (and with the same phase factor).*

Proof. Suppose $U(\tau)e_a = \gamma e_b$. Then

$$\gamma^{-1}e_a = U(-\tau)e_b$$

and if we take complex conjugate of both sides, we find

$$\gamma e_a = U(\tau)e_b,$$

as γ has norm 1. □

From now on, we may simply say that we have perfect state transfer *between* two vertices a and b, and in fact we might refer to this as *ab*-perfect state transfer. One consequence of this result is that, if we have *ab*-perfect state transfer at time t with phase factor γ, then

$$U(2t)e_a = U(t)^2 e_a = \gamma^2 e_a$$

and, similarly, $U(2t)e_b = \gamma^2 e_b$. We say that X is *periodic at u* if there is a time τ such that $U(\tau)e_a = \gamma e_a$ for some γ.

1.4.2 Corollary. *If we have perfect state transfer between a and b in X at time t, then X is periodic at a and at b, at time $2t$.* □

Although it is difficult to see any physical applications of periodicity, it provides a very useful mathematical tool for the analysis of perfect state transfer.

We say that a graph X is *periodic* if there is a time t such that $U(t)$ is diagonal. Equivalently X is periodic with period t at each vertex. By virtue of the following lemma, we do not need to make any assumptions on phase factors.

1.4.3 Lemma. *If X is connected and $U(t)$ is diagonal, then $U(t) = \gamma I$.*

Proof. If X is connected, the only diagonal matrices that commute with A are the scalar matrices. Since $U(t)$ and A commute, as we will see in the following sections, the lemma holds. □

If the eigenvalues of X are all integers it is easy to verify that X is periodic. It is a surprising fact that something very close to the converse is true, as we will see in Section 7.3.

1.5 Spectral Decomposition for Adjacency Matrices

Suppose A is a symmetric matrix with distinct eigenvalues $\theta_0, \dots, \theta_d$ and let E_r denote orthogonal projection onto the eigenspace belonging to θ_r, thus E_r is real, symmetric and idempotent. Moreover, E_r is a polynomial in A, and because A is diagonalizable, we have

$$\sum_{r=0}^{d} E_r = I.$$

As A is symmetric, its eigenspaces are orthogonal, and thus

$$E_r E_s = \delta_{r,s} E_r.$$

Finally

$$A = \sum_{r=0}^{d} \theta_r E_r;$$

this identity is known as the *spectral decomposition* of A. If f is an analytic function defined on the spectrum of A, then $f(A)$ is defined in terms of a power series, and

$$f(A) = \sum_{r=0}^{d} f(\theta_r) E_r.$$

All this is standard, see [28, Section 3.5] for example. It follows immediately that

$$U(t) = \exp(\mathrm{i}tA) = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} E_r,$$

and we shall use this identity extensively in the rest of this book. As each E_r is a polynomial in A, an immediate consequence is that $U(t)$ is a polynomial in A for all t, thus any matrix that commutes with A also commutes with $U(t)$.

If G is connected, the known Perron-Frobenius Theorem (see for instance [38, Chapter 8]) states that the largest eigenvalue of A is simple, and the matrix that represents orthogonal projection onto the corresdponding eigenspace has only positive entries. We shall typically assume θ_0 refers to the largest eigenvalue, thus the entries of E_0 are positive.

Another case of particular interest to us is the following identity:

$$(tI - A)^{-1} = \sum_{r=0}^{d} \frac{1}{t - \theta_r} E_r.$$

This allows us to express walk generating functions on a graph X in terms of its eigenvalues and the entries of the idempotents E_r. Thus

$$\frac{\phi(X \setminus u, t)}{\phi(X, t)} = \sum_{r=0}^{d} \frac{(E_r)_{u,u}}{t - \theta_r}.$$

where $\phi(X, t)$ is the characteristic polynomial of $A(X)$ in the variable t, and $X \setminus u$ is the graph obtained from X by removing the vertex u and the edges adjacent to it. We will take this up at length in Chapter 4.

By way of example, we compute the pieces in the spectral decomposition of P_3. The characteristic polynomial of P_3 is $t^3 - 2t$, whence its eigenvalues are

$$\sqrt{2}, \quad 0, \quad -\sqrt{2}.$$

The idempotents E_r (in the same order) are

$$\frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}, \qquad \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \qquad \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}.$$

In computing these it helps to note that if an eigenvalue is simple and z is an associated eigenvector with norm 1, then the projection E is equal to zz^T. In general the orthogonal projection onto an eigenspace of dimension m is simply the sum of the projections onto any set of m orthogonal one-dimensional subspaces.

1.6 Using Spectral Decomposition

So far the only graphs we have considered are P_2 and its Cartesian powers. To increase our range, we make extensive use of the spectral decomposition of symmetric matrices. If A is symmetric and has spectral decomposition

$$A = \sum_{r=0}^{d} \theta_r E_r$$

then

$$U(t) = \exp(\mathrm{i}tA) = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}\theta_r t} E_r.$$

From this we already see that $U(t)$ is a polynomial in A for any t, whence it commutes with A. Its eigenvalues are the numbers $\mathrm{e}^{\mathrm{i}\theta_r t}$.

By way of example, we apply this to the path P_3. Its spectral decomposition is computed at the end of Section 1.5. We have

$$U(t) = \mathrm{e}^{\mathrm{i}\sqrt{2}t} E_1 + E_2 + \mathrm{e}^{-\mathrm{i}\sqrt{2}t} E_3$$

and therefore

$$U(\pi/\sqrt{2}) = -E_1 + E_2 - E_3.$$

However

$$E_1 - E_2 + E_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

which is a permutation matrix and represents the automorphism of P_3 that swaps its end-vertices. It follows that we have perfect state transfer between the end-vertices of P_3 at time $\pi/\sqrt{2}$. We also have perfect state transfer on the Cartesian powers of P_3.

We can use the spectral decomposition of A to derive a factorization of $U(t)$. If

$$A = \sum_{r=0}^{d} \theta_r E_r,$$

then the summands commute and therefore

$$U(t) = \exp(\mathrm{i}tA) = \prod_{r=0}^{d} \exp(\mathrm{i}t\theta_r E_r).$$

If E is an idempotent, then $\mathrm{i}tE$ has the spectral decomposition

$$0 \cdot (I - E) + \mathrm{i}t \cdot E$$

and hence

$$\exp(\mathrm{i}tE) = I - E + \mathrm{e}^{\mathrm{i}t}E.$$

Thus we have the factorization

$$U(t) = \prod_{r=0}^{d} (I - E_r + \mathrm{e}^{\mathrm{i}\theta_r t} E_r).$$

Since $I - E_r + \mathrm{e}^{\mathrm{i}\theta_r t} E_r$ acts as the identity on the column space of $I - E_r$ and as multiplication by $e^{\mathrm{i}t\theta_r}$ (a complex number of norm one) on the column space of E_r, it might be viewed as a complex reflection about the subspace $\mathrm{col}(I - E_r)$. (A complex reflection relative to a subspace U fixes each vector in U and acts as multiplication by a complex scalar of norm one on $U^\perp$.)

1.7 Complete Graphs

The *complete graph* K_n is the graph on n vertices where all vertices are neighbours. The *complete bipartite graph* $K_{n,m}$ is the graph on $n+m$ vertices, where there is no edge amongst the first n vertices, no edge amongst the last m vertices, and otherwise all pairs of vertices are neighbours. It is a worthwhile exercise to show using the factorization in the end of last section that, in the complete bipartite graph $K_{2,n}$, we have perfect state transfer between the two vertices of degree n.

We introduce a useful and interesting bound, and apply it to complete graphs.

1.7.1 Lemma. *If X has spectral decomposition $\sum_r \theta_r E_r$ and $a, b \in V(X)$, then*

$$|U(t)_{a,b}| \leq \sum_{r=0}^{d} |(E_r)_{a,b}|.$$

Proof. We apply the triangle inequality to

$$U(t) = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} E_r,$$

noting that all eigenvalues have norm 1. □

We will study this inequality in greater depth in Section 7.1. For now, we apply it to the complete graphs. Note first that $A(K_n) = J - I$ where J is the all 1s matrix of appropriate size. It is a simple exercise to show that the eigenvalues of K_n are $n-1$ (which is simple) and -1 (with multiplicity $n-1$). The corresponding idempotents are

$$\frac{1}{n}J, \qquad I - \frac{1}{n}J$$

and consequently

$$U(t) = \mathrm{e}^{\mathrm{i}(n-1)t}\frac{1}{n}J + \mathrm{e}^{-\mathrm{i}t}\left(I - \frac{1}{n}J\right).$$

The bound in Lemma 1.7.1 yields that if a and b are distinct vertices in K_n, then

$$|U(t)_{a,b}| \leq \frac{2}{n}.$$

This implies immediately that the only complete graph with perfect state transfer is K_2, which happens to be equal to P_2. If we have uniform mixing on K_n at time t, then each off-diagonal entry of $U(t)$ has absolute value equal to $1/\sqrt{n}$. However if

$$\frac{1}{\sqrt{n}} \leq \frac{2}{n}$$

then $n \leq 4$, and so uniform mixing cannot occur on K_n if $n > 4$, despite what our intuition might suggest. In fact, a quantum walk on K_n tends to stay at the start vertex, which already displays a significant contrast to the classical case.

1.8 Bipartite Graphs

A *bipartite graph* is a graph where the vertex set can be partitioned into two classes, and all edges of the graph have one end in each class. Note that two vertices in the same class are at even distance, and two vertices in opposite classes are at odd distance. The entries of $U(t)$ are complex numbers with norm at most 1. When X is bipartite though we can say more.

Assume X is bipartite on n vertices. We can always order the vertices in such way that the adjacency matrix has the following form:

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

where B is a 01-matrix of appropriate size.

1.8.1 Lemma. *Assume X is bipartite and A has partitioned form*

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

Then there are real symmetric matrices $C_1(t)$ and $C_2(t)$, and a real matrix $K(t)$ such that

$$U(t) = \begin{pmatrix} C_1(t) & \mathrm{i}K(t) \\ \mathrm{i}K(t)^T & C_2(t) \end{pmatrix}.$$

Proof. If

$$D := \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

then $DAD = -A$. Consequently

$$DU(t)D = U(-t) = \overline{U(t)},$$

which implies that the diagonal blocks of $U(t)$ are real and the off-diagonal blocks are purely imaginary. Since $U(t)$ is symmetric, so are C_1 and C_2. □

As an exercise, you might prove that

$$C_1(t) = \cos(t\sqrt{BB^T}), \qquad C_2(t) = \cos(t\sqrt{B^TB}).$$

What we are seeing in the above expression for $U(t)$ is a reflection of the fact that $U(t)$ is normal and any normal matrix can be written as a sum $C + \mathrm{i}S$ where C and S are commuting Hermitian matrices. (If N is normal, then $C = \frac{1}{2}(N+N^*)$ and $S = \frac{1}{2\mathrm{i}}(N-N^*)$ are commuting Hermitian matrices.)

This simplification of the form of $U(t)$ still holds if we allow B to be a weighted adjacency matrix, but not if we use the Laplacian (because then the diagonal is not zero).

The above considerations lead to the following result, due to Kay [45, Section III].

1.8.2 Lemma. *Let X be a bipartite graph. If we have perfect state transfer from u to v at time t, then the phase factor is ± 1 if $\operatorname{dist}(u,v)$ is even, and is $\pm \mathrm{i}$ if $\operatorname{dist}(u,v)$ is odd.* □

We shall return to perfect state transfer on bipartite graphs later.

1.9 Uniform Mixing on Bipartite Graphs and Hadamard matrices

A Hadamard matrix H is a square $n \times n$ matrix whose all entries are equal to ± 1, and such that

$$HH^T = nI.$$

Hadamard matrices have been studied for more than 100 years. It is easy to see that

$$H = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

is a Hadamard matrix, and so are all matrices $H^{\otimes k}$ for $k \geq 2$. If H is a $n \times n$ Hadamard matrix with $n \geq 3$, then it is well known that $n \equiv 0 \pmod 4$. It is a major open problem in combinatorics to decide whether or not a $n \times n$ Hadamard matrix exists for all $n \equiv 0 \pmod 4$. We use the term *complex Hadamard matrix* to refer to a matrix H such that $HH^T = nI$, and all entries of H are ± 1 or $\pm \mathrm{i}$.

We use the results of the previous section to derive some useful information concerning uniform mixing on bipartite graphs, and to establish a connection between quantum walks and Hadamard matrices. Recall that a graph X admits uniform mixing at time t if $U(t)$ is a flat complex matrix.

1.9.1 Theorem. *Let X be a bipartite graph on n vertices. If uniform mixing occurs on X then $n = 2$ or n is divisible by four; if X is regular and uniform mixing occurs then n is the sum of two squares.*

Proof. Assume X is bipartite and $U(t)$ is flat for some t. As we have seen, each entry of $U(t)$ is either real or purely imaginary, and it follows that $\sqrt{n}U(t)$ must be a complex Hadamard matrix with entries ± 1 and $\pm i$. Let D be a diagonal matrix with $D_{u,u} = 1$ if u is in the first class of the bipartition of X, and $D_{u,u} = \mathrm{i}$ otherwise. Then

$$D^*U(t)D = \begin{pmatrix} C_1(t) & -K(t) \\ K(t)^T & C_2(t) \end{pmatrix}$$

where $C_1(t)$, $C_2(t)$ and $K(t)$ are real matrices. Therefore $\sqrt{n}D^*U(t)D$ is a real Hadamard matrix, and thus $n = 2$ or n is divisible by four.

If X is regular then the all-ones vector $\mathbf{1}$ is an eigenvector of A. As $U(t)$ is a polynomial in A, it follows that there are integers a and b such that

$$\sqrt{n}U(t)\mathbf{1} = (a + \mathrm{i}b)\mathbf{1};$$

taking complex conjugates yields that

$$\sqrt{n}U(-t) = (a - \mathrm{i}b)\mathbf{1}$$

and consequently

$$(a - ib)(a + ib)\mathbf{1} = nU(-t)U(t)\mathbf{1} = n\mathbf{1}. \qquad \square$$

An even cycle is regular and bipartite, so the above result provides another proof of some results of Adamczak et al [1]. Carlson et al [17] proved that uniform mixing does not occur on C_5. In Chapter 17 we will see that there is no uniform mixing on even cycles of length greater than four, and no uniform mixing on the cycles C_p, where p is a prime greater than three.

1.10 Cospectral and Strongly Cospectral Vertices

If we have perfect state transfer from vertex a to b, what properties must a and b share. Could they have different valency? We use the spectral decomposition to derive constraints.

1.10.1 Lemma. *Let $A = \sum_r \theta_r E_r$ be the spectral decomposition of X. If we have perfect state transfer from a to b, then:*

(a) For each for each non-negative integer k we have $(A^k)_{a,a} = (A^k)_{b,b}$.

(b) For each for each r we have $(E_r)_{a,a} = (E_r)_{b,b}$.

Proof. If we have perfect state transfer from a to b at time t, there is a complex number γ with norm one such that

$$U(t)e_a = \gamma e_b$$

and, since $U(t)$ commutes with powers of A,

$$U(t)A^k e_a = \gamma A^k e_b.$$

Hence

$$(A^k)_{b,b} = \langle e_b, A^k e_b\rangle = \langle \gamma^{-1}U(t)e_a, \gamma^{-1}U(t)A^k e_a\rangle.$$

Since U is unitary and $\|\gamma\| = 1$,

$$\langle \gamma^{-1}U(t)e_a, \gamma^{-1}U(t)A^k e_a\rangle = \langle e_a, A^k e_a\rangle = (A^k)_{a,a}.$$

Now we note that each spectral idempotent is a polynomial in A, and so (b) follows at once. □

Since $(A^2)_{u,u}$ is the valency of the vertex u, it follows that if we have perfect state transfer from a to b, then a and b have the same valency. More generally, for each integer k, the number of closed walks of length k on a equals the number on b. (So, for example, the number of triangles on a is equal to the number on b.) If condition (a) holds for vertices a and b, we say that they are *cospectral*.

If $U(t)e_a = \gamma e_b$, then

$$\gamma E_r e_b = U(t)E_r e_a = e^{\mathrm{i}t\theta_r} E_r e_a$$

and hence

$$E_r e_b = \gamma^{-1} e^{\mathrm{i}t\theta_r} E_r e_a.$$

As both $E_r e_b$ and $E_r e_a$ are real, $e^{\mathrm{i}t\theta_r} E_r e_a$ is real and, since $\|\gamma^{-1}e^{\mathrm{i}t\theta_r}\| = 1$, we have the following.

1.10.2 Lemma. *If there is perfect state transfer from a to b, then $E_r e_b = \pm E_r e_a$ for each r.* □

If we have $E_r e_b = \pm E_r e_a$ for each r, we say that the vertices a and b are *strongly cospectral*.

We leave it as an exercise to show that if $(E_r)_{a,a} = (E_r)_{b,b}$ for each r, then a and b are cospectral.

We treat cospectral and strongly cospectral vertices at (much) greater length in Chapter 6.

1.11 Vertex-Transitive Graphs

Suppose we have perfect state transfer from a to b in X. Then

$$U(t)e_a = \gamma e_b$$

for some complex number γ with $|\gamma| = 1$, and, since A commutes with $U(t)$ we get

$$U(t)Ae_a = \gamma Ae_b.$$

Since $U(t)$ is unitary and $\|\gamma\| = 1$, we see that $\|Ae_a\|^2 = \|Ae_v\|^2$. Thus a and b have the same valency, and this also indicates that if we have perfect state transfer from a to b, then a and b should be somehow similar. This suggests that vertex-transitive graphs would be a good place to look for perfect state transfer. In this section give some thought to the connection between vertex transitivity and state transfer.

An *automorphism* of a graph X is a bijection $f : V(X) \to V(X)$ that maps adjacent pairs of vertices to adjacent pairs. A bijection from a finite set on n elements to itself is a permutation, and provided that the elements of the set are somehow ordered, say $\{a_1, ..., a_n\}$, each permutation π corresponds uniquely to a 01-matrix P defined as $P_{ij} = 1$ if and only if $\pi(a_i) = a_j$. It is an enlightening exercise to verify that a permutation π is an automorphism of a graph if and only if its corresponding matrix P commutes with $A(X)$. (Provided, of course, that the same ordering is used to construct P and A.)

The permutation matrices that commute with A form a group of matrices isomorphic to the automorphism group of X. (The latter consists of permutations of $V(X)$ and the former consists of matrices; it is usually simplest to ignore the difference, and refer to either presentation as $\mathrm{Aut}(X)$.)

The vertex set of X is partitioned into orbits of the action of $\mathrm{Aut}(X)$. When there is only one orbit, the graph is *vertex transitive*. In a vertex transitive graph, for any two vertices a and b, there is always a permutation matrix P that commutes with A so that $Pe_a = e_b$.

Suppose we have perfect state transfer from a to b in a vertex-transitive graph X. Assume $U(\tau)e_a = \gamma e_b$. If the permutation matrix P commutes with A, it must commute with $U(t)$, and then

$$\gamma Pe_b = PU(\tau)e_a = U(\tau)Pe_a.$$

Hence if have perfect state transfer from a to b at time τ, then we have perfect state transfer from the image of a under P to the image of b. Consequently there is a partition of $V(X)$ into pairs and at time τ we have perfect state transfer between each vertex and its partner, all happening with the same complex number γ. Accordingly there is a permutation matrix T such that

$$U(\tau) = \gamma T;$$

further all diagonal entries of T are zero and $T^2 = I$. Since T must commute with A it is an automorphism of X. Since $U(t)$ commutes with $\mathrm{Aut}(X)$, it follows that T lies in the center of $\mathrm{Aut}(X)$.

1.11.1 Theorem. *Assume X is a vertex-transitive graph. If at time τ we have perfect state transfer from a to b, then there is a complex number γ and a permutation matrix T such that $U(\tau) = \gamma T$. The permutation matrix T is a fixed-point free automorphism of X with order two that lies in the center of* $\mathrm{Aut}(X)$. □

We point out that this result also holds if X has multiple edges or loops, the key to the argument is that $U(\tau)$ must commute with each element of $\mathrm{Aut}(X)$.

1.11.2 Corollary. *If a vertex-transitive graph admits perfect state transfer, then $V(X)$ is even.* □

1.12 Pretty Good State Transfer

We have already discussed two types of phenomena that could happen in a quantum walk at a fixed time. Perfect state transfer and uniform mixing are both defined when the absolute values of certain entries of $U(t)$ attain, respectively, 1 or $1/\sqrt{n}$. We will see later that a quantum walk on a graph has a somewhat oscillating and periodic or almost periodic behavior. So there makes no sense to ask if it could be that $|U(t)_{ab}|$ tends to 1 or $1/\sqrt{n}$ or any other value as $t \to \infty$. But we can and will ask if there is a set of distinct times $t_0 < t_1 < t_2 < \ldots$ so that $(|U(t_k)_{ab}|)_{k \geq 0}$ converges. In this section, we introduce our first example.

We say a graph X admits *pretty good state transfer* from a to b if for any $\varepsilon > 0$, there is a $t \in \mathbb{R}$ such that

$$|U(t)_{a,b}| > 1 - \varepsilon.$$

It is not hard to see that if we have pretty good state transfer from a to b, we must also have pretty good state transfer from b to a. We view pretty good state transfer as an interesting and possibly useful approximation to perfect state transfer. We provide an example of the concept by showing that it occurs on P_4 while perfect state transfer does not.

The eigenvalues of P_4 are

$$\theta_1 = \frac{1}{2}(\sqrt{5}+1), \quad \theta_2 = \frac{1}{2}(\sqrt{5}-1), \quad \theta_3 = \frac{1}{2}(-\sqrt{5}+1), \quad \theta_4 = \frac{1}{2}(-\sqrt{5}-1).$$

and by straightforward computation we find that

$$E_1 - E_2 + E_3 - E_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Denote the matrix on the right by R. (We could prove that $R = \sum_r (-1)^{r-1} E_r$ by verifying that if z_r is an eigenvector with eigenvalue θ_r, then $Rz_r = (-1)^{r-1} z_r$, for all paths. Verifying all these details right now is not trivial, but everything we need is covered in Chapter 10.)

Now choose integers p and q so that

$$\frac{p}{q} \approx \frac{1+\sqrt{5}}{2}.$$

Then $q\theta_1 \approx p$ and

$$q\theta_2 = q(\theta_1 - 1) \approx p - q, \quad q\theta_3 \approx q - p, \quad q\theta_4 \approx -p.$$

For example take $p = 987$ and $q = 610$ and set $\tau = 610\pi/2$. Then the values of $\tau\theta_r$ are (approximately)

$$987\pi/2, \quad 377\pi/2, \quad -377\pi/2, \quad -987\pi/2$$

and these are congruent modulo 2π to

$$3\pi/2, \quad \pi/2, \quad 3\pi/2, \quad \pi/2.$$

Hence

$$U(305\pi) \approx -iR.$$

(The approximation is accurate to five decimal places.)

In general we have to choose p and q so that $p \equiv 3$ and $q \equiv 2$ modulo 4. If f_n is the n-th Fibonacci number with $f_0 = f_1 = 1$ then

$$f_{4m+2} \equiv 2 \pmod 4 \quad \text{and} \quad f_{4m+3} \equiv 3 \pmod 4,$$

and the ratios f_{n+1}/f_n are the standard continued fraction approximation to $(1+\sqrt{5})/2$. We conclude that we have pretty good state transfer between the end-vertices of P_4. We leave the reader the exercise of verifying that there is also pretty good state transfer between the end-vertices of P_5 (for which the eigenvalues are 0, ± 1, $\pm\sqrt{3}$).

In Section 10.6 we will see that we do **not** have perfect state transfer on P_n when $n \geq 4$. If Chapter 11 we return to the study of pretty good state transfer on paths. There we will see many cases where it occurs, but we will also see that to get a good approximation to perfect state transfer, we usually need the time t to be very large. This suggests that pretty good state transfer will not be a satisfactory substitute for perfect state transfer in practice.

1.13 Oriented Graphs

An *oriented graph* is a directed graph where each pair of distinct vertices is joined by at most one arc. If B is the adjacency matrix of an oriented graph, then $B \circ B^T = 0$ (which we could take to be the definition), and the graph is determined by the signed matrix $B - B^T$, which we call the *signed adjacency matrix* of the oriented graph. One advantage of the signed matrix is that it is skew symmetric and hence normal, and so we can hope for useful relations between the eigenvalues and the combinatorial properties of the oriented graph. A tournament is an oriented complete graph. We note that an induced subgraph of an oriented graph is again an oriented graph.

If A is skew symmetric, the matrices

$$U(t) := \exp(tA), \qquad (t \in \mathbb{R})$$

are orthogonal—just check:

$$(\exp(tA))^T = \exp(tA^T) = \exp(-tA).$$

Hence $U(t)$ defines a continuous quantum walk on the vertices of the oriented graph. Since the entries of $U(t)$ are real, it might seem strange to refer to this as a 'quantum walk'. But the entries of $U(t)$ cannot be all non-negative unless $A = 0$, so it is not a classical random walk and, in any case, it is the mixing matrix $M(t)$ which predicts the observable behaviour of the walk and this matrix if real even for our usual walks.

The idea of studying continuous walks on oriented graphs, and the basic theory, are due to Cameron et al. [16].

Skew-symmetric matrices are normal, and so have a spectral decomposition. We work out spectral decomposition for oriented graphs. Note that if $A^T = -A$, then $(iA)^* = iA$, whence we see that A is skew symmetric if and only if $-iA$ is Hermitian.

1.13.1 Lemma. *If $A^T = -A$, then all eigenvalues of A are purely imaginary and the spectrum of A is closed under multiplication by -1. If θ is an eigenvalue of A with spectral projection E, then projection belonging to $-\theta$ is $E^T = \overline{E}$.*

Proof. As iA is Hermitian, we have the spectral decomposition

$$iA = \sum_r \theta_r E_r$$

where the eigenvalues θ_r are real and the idempotents E_r are Hermitian. Therefore all eigenvalues of A have real part zero.

If λ is a nonzero eigenvalue of A with associated idempotent E, then $AE = \lambda E$ and therefore

$$A\overline{E} = \overline{A}\overline{E} = \overline{\lambda}\overline{E}.$$

This implies that $\overline{E}_r$ is the spectral idempotent corresponding to the complex conjugate of θ_r. But $\bar{\theta}_r = -\theta_r$, and so the rest of our claims follow. □

For a second approach, note that if A is skew-symmetric it is normal and so there is a unitary matrix L and a diagonal matrix Δ such that $A = L\Delta L^*$. Now

$$-A = A^T = A^* = L\overline{\Delta}L^*$$

and therefore $\overline{\Delta} = -\Delta$.

It follows that we can write

$$A = \sum_{r:\theta_r>0} i\theta_r(E_r - \overline{E}_r).$$

where $i(E_r - \overline{E}_r)$ is real and skew symmetric and

$$(E_r - \overline{E}_r)^2 = E_r + \overline{E}_r.$$

If $r \neq s$, then

$$(E_r - \overline{E}_r)(E_s - \overline{E}_s) = 0.$$

Using the spectral decomposition of $U(t)$, we have

$$U(t) = \sum_r e^{it\theta_r} E_r = E_0 + \sum_{r:\theta_r>0} \cos(\theta_r t)(E_r + \overline{E}_r) + \sum_{r:\theta_r>0} \sin(\theta_r t)(iE_r - i\overline{E}_r)$$

where, despite appearances, each term in the last summand is real. Note that this identity expresses $U(t)$ as the sum of commuting symmetric and skew symmetric matrices.

We say vertices a and b in an oriented graph are *strongly cospectral* if for each idempotent E_r there is a complex scalar γ_r such that $\|\gamma_r\| = 1$ and $E_r e_a = \gamma_r E_b$.

1.13.2 Lemma. *If all vertices in the oriented graph X are strongly cospectral, than all eigenvalues of the signed adjacency matrix of X are simple.*

Proof. The eigenspace belonging to the eigenvalue θ_r is spanned by the projections $E_r e_a$ for a in $V(X)$. If each two of these vectors are parallel, their span is 1-dimensional. □

1.14 Multiple State Transfer

Lemma 1.4.1 tells us that if we have perfect state transfer from a to b in a continuous walk at time t, then we also have perfect state transfer from b to a at time t. We will also see (Corollary 7.8.2) that if we have perfect state transfer from a to b in a continuous walk, then at no time is there perfect state transfer from a to a vertex distinct from b. For walks on oriented graphs, the situation is quite different.

We consider the walk on the cyclic orientation of K_3 with adjacency matrix

$$A = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}.$$

Define the permutation matrix P to be

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

so $A = P - P^T$. Set

$$\omega = \frac{1}{2}(-1 + i\sqrt{3}).$$

The eigenvectors of P are

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ \omega \\ \omega^2 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ \omega^2 \\ \omega \end{pmatrix}$$

with respective eigenvalues

$$1, \quad \omega, \quad \omega^2.$$

As

$$\omega = \frac{1}{2}(-1 + i\sqrt{3}),$$

we have

$$\omega - \omega^2 = i\sqrt{3}.$$

and the eigenvalues of A are 0, $i\sqrt{3}$ and $-i\sqrt{3}$.

The spectral idempotents of P are the matrices zz^* where z runs over the normalized eigenvectors of P. Thus they are

$$\frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \frac{1}{3}\begin{pmatrix} 1 & \omega^2 & \omega \\ \omega & 1 & \omega^2 \\ \omega^2 & \omega & 1 \end{pmatrix}, \quad \frac{1}{3}\begin{pmatrix} 1 & \omega & \omega^2 \\ \omega^2 & 1 & \omega \\ \omega & \omega^2 & 1 \end{pmatrix}.$$

and therefore the spectral decomposition of $U(t)$ is

$$U(t) = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{e^{it\sqrt{3}}}{3}\begin{pmatrix} 1 & \omega^2 & \omega \\ \omega & 1 & \omega^2 \\ \omega^2 & \omega & 1 \end{pmatrix} + \frac{e^{-it\sqrt{3}}}{3}\begin{pmatrix} 1 & \omega & \omega^2 \\ \omega^2 & 1 & \omega \\ \omega & \omega^2 & 1 \end{pmatrix}$$

If $\tau := \frac{2\pi}{3\sqrt{3}}$ then

$$e^{i\tau\sqrt{3}} = e^{2\pi i/3} = \omega$$

and consequently

$$(U(\tau))_{1,2} = 1.$$

Since $U(\tau)$ is unitary and a circulant, we have proved that

$$U(\tau) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

1.14.1 Lemma. *Let $U(t)$ be the continuous quantum walk on the cyclic orientation of K_3. Then we have perfect state transfer from vertex 1 to vertex 2 at time $\frac{2\pi}{3\sqrt{3}}$, and perfect state transfer from vertex 1 to vertex 3 at time $\frac{4\pi}{3\sqrt{3}}$.*

Proof. As

$$U(\tau) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

it follows that

$$U(2\tau) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}^2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$ □

This example is due to Tamon et al []. They say that the cyclic orientation of K_3 admits *universal perfect state transfer*, since there is perfect state transfer between any two distinct vertices.

An oriented graph admits *multiple state transfer* if there a vertex that admits perfect state transfer to two distinct vertices. One way to achieve this is to choose the oriented graph and the time such that $U(t)$ is a monomial matrix. Since the Kronecker products of monomial matrices is a monomial matrix, the Cartesian powers of the cyclic orientation of K_3 provide an infinite family of examples with multiple state transfer.

1.15 Path Plots

Here we plot the probability of transfer between the end vertices of paths.

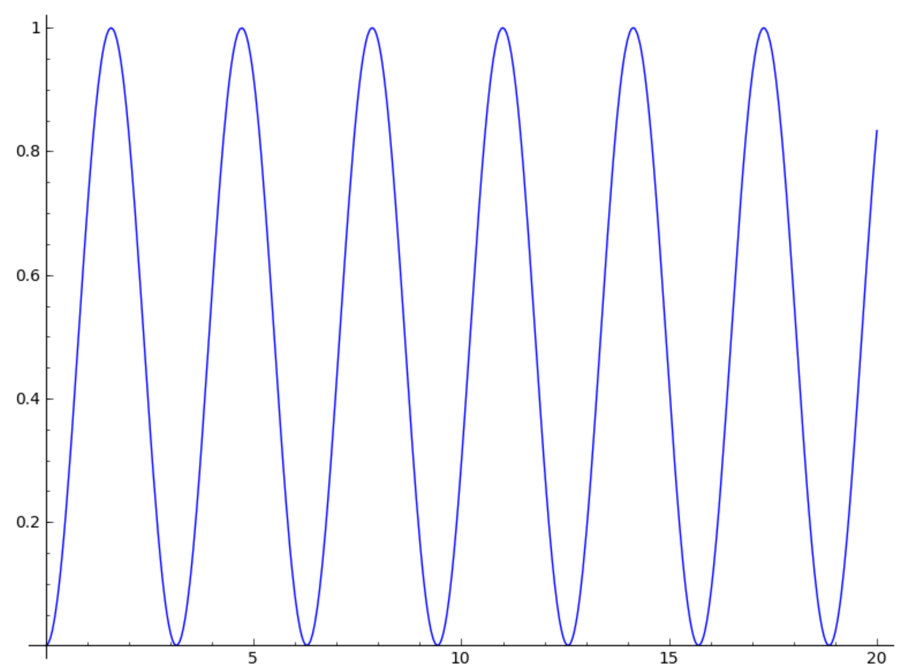

Figure 1.3: P_2: $M(t)_{0,1}$

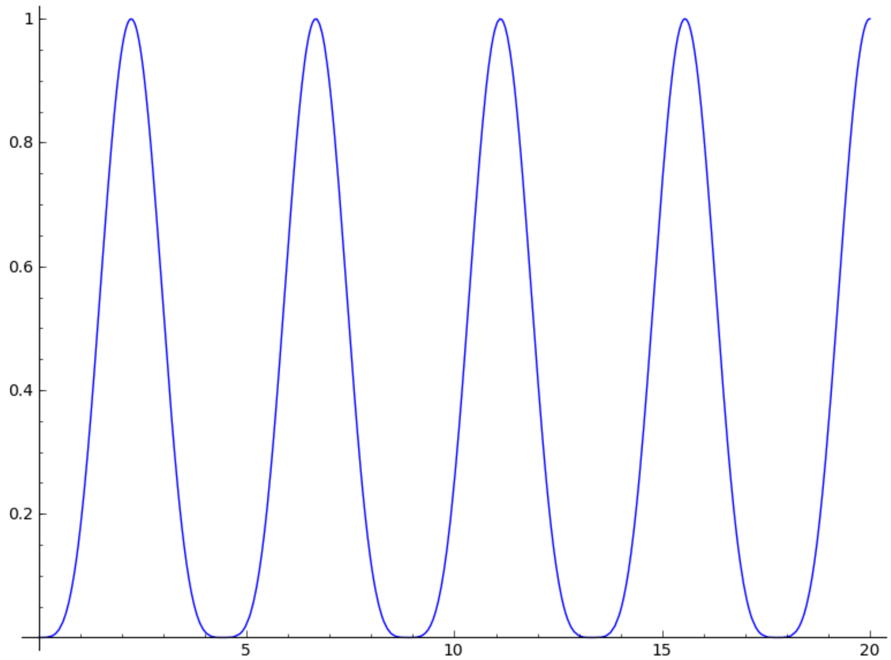

Figure 1.4: P_3: $M(t)_{0,2}$

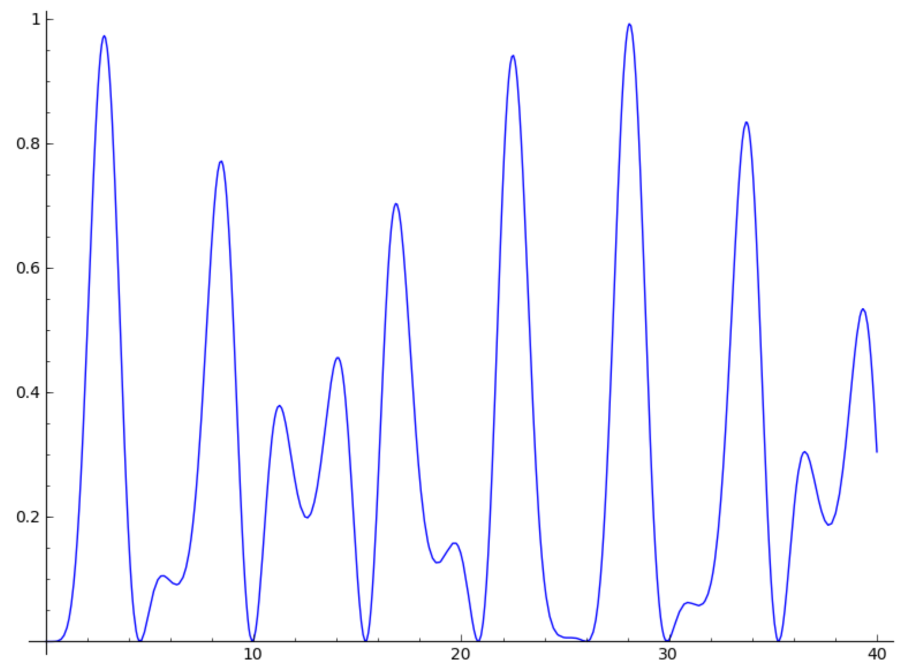

Figure 1.5: P_4: $M(t)_{0,3}$

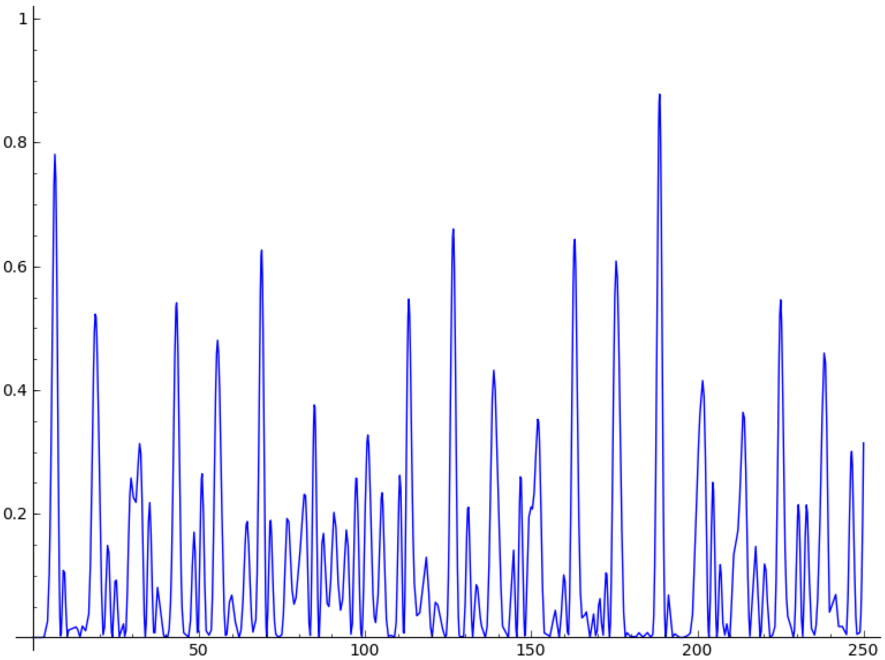

Figure 1.6: P_{11}: $M(t)_{0,10}$

1.16 One More Plot

Here is a plot in the complex plane of $U_{C_5}(t)_{0,1}$ as a function of time. One question is whether this entry is zero at some positive value of t.

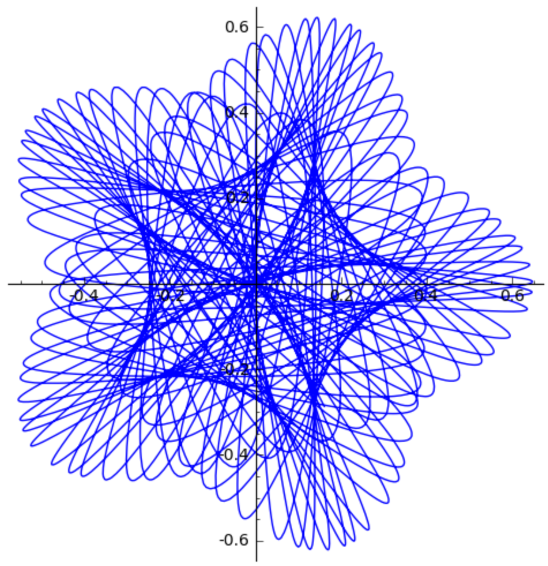

Figure 1.7: C_5: $U(t)_{0,1}$

Notes

Continuous quantum walks were introduced by Farhi and Gutmann in [29]. The concept of state transfer first appears in [12] and the basic theory of perfect state transfer was mapped out by Christandl et al. in [20]. In particular the latter paper shows that perfect state transfer occurs on P_2 and P_3, and on their Cartesian powers. It also offers a proof that, if $n > 3$, we do not have perfect state transfer between the end-vertices of P_n. (We will consider this in Section 10.6, where we prove that we do not have perfect state transfer between any two vertices of P_n when $n > 3$.) We provide a deeper treatment of perfect state transfer in Chapter 7.

Uniform mixing (or instantaneous uniform mixing) appears first in work of Moore and Russell [48]. We return to this topic in Chapter 17, related ideas will be taken up there and in Chapter 15.

Exercises

1-1. Show that in the complete bipartite graph $K_{2,n}$, we have perfect state transfer between the vertices of degree n.

1-2. Show that we do have uniform mixing on K_2, K_3 and K_4.

1-3. Show that if A and B commute, then $\exp(A+B) = \exp(A)\exp(B)$.

1-4. Let $\overline{X}$ be the complement of a regular graph X on n vertices, that is, $\overline{A} = A(\overline{X}) = J - I - A(X)$. Show that at times t which are integers multiples of $2\pi/n$, $\exp(\mathrm{i}t\overline{A})$ and $\exp(\mathrm{i}tA)$ are very much alike.

1-5. Show that we have perfect state transfer on $\overline{nK_2}$ when n is even, and on $\overline{nC_4}$ for all n. (Here and elsewhere we use nX to denote the union of n vertex-disjoint copies of X.)

1-6. Show that if $(E_r)_{a,a} = (E_r)_{b,b}$ for each r, then a and b are cospectral. Hence deduce that if vertices a and b are strongly cospectral, they are cospectral.

1-7. Suppose X is bipartite with adjacency matrix

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

and

$$U(t) = \begin{pmatrix} C_1(t) & \mathrm{i}K(t) \\ iK(t)^T & C_2(t) \end{pmatrix}.$$

Prove that

$$C_1(t) = \cos(t\sqrt{BB^T}), \qquad C_2(t) = \cos(t\sqrt{B^TB}).$$

1-8. Prove that any two vertices in a vertex-transitive graph are cospectral.

1-9. Show that no two vertices of the Petersen graph are strongly cospectral. [Warning: with only the information at hand, this is hard; it is a consequence of results we prove later.]

1-10. What can you say about instantaneous uniform mixing on $\overline{nK_2}$ and on $\overline{nC_4}$?

1-11. Show that pretty good state transfer occurs (according to the official definition given) if and only if there is an *increasing* sequence $(t_k)_{k\geq 0}$ such that

$$\lim_{k\to\infty} |U(t_k)_{a,b}| = 1.$$

(This will be a nice review of the first part of your first real analysis course.)

Chapter 2

Physics

In this chapter we lay the foundations for the quantum information theory that we will need later in the text. By no means do we intend this to be a conceptual, well motivated and detailed introduction to either quantum physics or quantum information theory. Our aims, rather, are quite modest and almost mundane. We present nomenclature, definitions and notation. The objects and their properties will be defined solely using mathematical language. (Proper references will be provided in the Notes, at the end of the chapter.)

We have chosen not to use Dirac's bra-ket notation. So we will take the standard basis for $\mathbb{C}^2$ to consist of vectors f_0 and f_1. If M and N are complex matrices of the same order, we define

$$\langle M, N \rangle = \operatorname{tr}(M^* N) = \operatorname{sum}(\overline{M} \circ N);$$

this is an inner product on $m \times n$ matrices.

2.1 Quantum Systems

Quantum mechanics is founded on a set of axioms which describe the mathematics behind its nature. We offer a description here which would be in line with a standard introductory course in quantum physics. In the following sections, we offer a description that is more in line with the standard usage in quantum information theory.

The state of a quantum system is a 1-dimensional subspace of a Hilbert space. Our systems will always be finite-dimensional, so our underlying vector space is $\mathbb{C}^m$ with the standard complex inner product, for some natural m. A quantum system with dimension two is known as a *qubit*. Any complex vector space gives rise to a complex projective space, and the *states* of a quantum system can be seen as the points of this projective space, or, alternatively, they are lines in $\mathbb{C}^m$.

There are two customary ways of representing states. The first is to choose a unit vector that spans the line of interest, and in this case there are an infinite number of choices, as the underlying field is $\mathbb{C}$. The second is to give the matrix that represents the orthogonal projection onto the line. If z is a unit vector, the projection onto the line it spans is $P = zz^*$. Note that if $\lambda \in \mathbb{C}$ and $|\lambda| = 1$ then

$$(\lambda z)(\lambda z)^* = \lambda\bar{\lambda}zz^* = zz^*.$$

This reflects the fact that the matrix representing orthogonal projection onto a subspace does not depend on the choice of basis for the subspace. From here on and throughout the whole text, we shall usually prefer to represent a quantum state by its associated rank one projector.

Two quantum systems can be composed. **The state space of their composition is the tensor product of their individual state spaces.** In other words, a *compound quantum system* is represented by the tensor product of simple systems. So $(\mathbb{C}^2)^{\otimes d}$ corresponds to a system of d qubits, and such a system will be the heart of any quantum computer, as a qubit can effectively be realized as a physical object, and so can their composition.

We saw an example of this in Section 1.2, where we proved that

$$U_{X\square Y}(t) = U_X(t) \otimes U_Y(t).$$

Here the right side acts on $\mathbb{C}^{V(X)} \otimes \mathbb{C}^{V(Y)}$, which is a composite system. We could view this as formed from two independent quantum walks, one on X and the other on Y. Thus a continuous walk on a complicated graph (the Cartesian product) can be viewed as the composite of two walks on simpler graphs.

The time-evolution of a *closed* quantum system is determined by a unitary mapping on $\mathbb{C}^m$. So if our system state is represented by the vector z and it evolves and changes, the state of the new system will be Uz, for some unitary matrix U. If $P = zz^*$, then the evolution takes P to UPU^*. The matrix U might be a function of time, and for a continuous quantum walk, we typically have $U = U(t) = \exp(\mathrm{i}tH)$, for some Hermitian matrix H.

The axioms also describe which properties can be "observed" or measured in a quantum system. **The *observables* of a quantum system $\mathbb{C}^m$ are the self-adjoint operators acting on this system, that is, they correspond to the Hermitian matrices.** Assume an observable H admits spectral decomposition

$$H = \sum_{r=1}^{k} \lambda_r F_r.$$

If the system is in a state described by the rank-1 projection P, then, after carrying out a *projective measurement* with respect to the observable H, the axioms of quantum mechanics tells us two things:

(i) with probability $\langle F_r, P\rangle$, the result of the measurement is λ_r;

(ii) if the result of the measurement is λ_r, then the state of the system changes to a state described by

$$\frac{1}{\langle F_r, P\rangle} F_r P F_r.$$

Generally physicists choose their Hermitian operators to have only simple eigenvalues, and so the eigenspaces can be specified by giving an orthonormal basis of $\mathbb{C}^m$. In the context of quantum computing, we usually assume that the orthogonal basis is the standard basis for our vector space.

It is important to realize that a measurement does not reveal the "true" state of the system. Rather, it imposes a state on the system.

2.2 Density Matrices and POVMs

We now offer a second description of the basics of quantum physics; this is more in line with the viewpoint usually taken in quantum computing. Our second approach may seem more general, but it is equivalent to the first.

A *state* is represented by a positive semidefinite matrix with trace one, such matrices are called *density matrices*. If z is a non-zero vector in $\mathbb{C}^d$, the line spanned by z is determined by the projection

$$P = \frac{1}{z^* z} z z^*.$$

Here P is positive semidefinite and $\operatorname{tr}(P) = 1$, so P is a density matrix. In this case $\operatorname{rk}(P) = 1$. We will say that a density matrix with rank one specifies a *pure state*. A general density matrix is referred to as a *mixed state*. Our next result explains the terminology.

2.2.1 Lemma. *If Q is positive semidefinite and $\operatorname{tr}(Q) = 1$, then Q can be written as a convex combination of positive semidefinite matrices of rank 1.*

Proof. If $\operatorname{rk}(Q) = k$, we can find an orthonormal set $x_1, \dots, x_k$ of eigenvectors for Q with respective non-zero eigenvalues $\lambda_1, \dots, \lambda_k$. Then

$$Q = \sum_{r=1}^{k} \lambda_r x_r x_r^*$$

and since the eigenvalues of Q are nonnegative and sum to 1, we are done. □

It wil be possible to express Q as a convex combination of pure states in many different ways—the pure states are not determined by Q. The set of $d \times d$ density matrices is a compact convex set, and it follows from the previous lemma that the pure states are its extreme points.

We turn to measurements. A *measurement* is given by a sequence $M_1, \dots, M_e$ of positive semidefinite matrices such that $\sum_r M_r = I$. Such a sequence is called a *positive operator-valued measurement*, and is referred to by the acronym *POVM*. A measurement is *projective* if each element M_i is a projection. Thus the measurements described in the previous section are projective. (However the matrices in a projective measurement are not required to have rank one.)

The outcome of a measurement is an element of the the index set $\{1, \dots, e\}$ and if the state is given by the density matrix D, the probability that we observe outcome i is

$$\langle M_i, D \rangle = \operatorname{tr}(M_i D).$$

Recall that if M and D are positive semidefinite matrices of the same order, then $\langle M, D \rangle \geq 0$, and equality holds if and only if $MD = 0$. So $\langle M_i, D \rangle \geq 0$ and, since $\sum M_i = I$, we have

$$\sum_i \langle M_i, D \rangle = \langle \sum_i M_i, D \rangle = \langle I, D \rangle = \operatorname{tr}(D) = 1.$$

Hence, given D, the POVM $M_1, \dots, M_e$ defines a probability density on $\{1, \dots, e\}$.

The combination of density matrix and POVM does not suffice to determine the post-measurement state. This is not a problem—many physical measurements destroy the state of the system, and in that case it does not even make sense to speak of a post-measurement state.

If H is a Hermitian matrix and $E_1, \ldots, E_m$ are the idempotents in the spectral decomposition of H, then they form a POVM. The simplest case is when the eigenvalues of H are simple, when there is an orthonormal basis $z_1, \ldots, z_d$ (consisting of eigenvectors for H) and $E_i = z_i z_i^*$. Then

$$\langle E_i, D\rangle = \operatorname{tr}(E_i D) = \operatorname{tr}(z_i z_i^* D) = z_i^* D z_i;$$

if moreover D is a pure state, say $D = xx^*$ for a unit vector x, then

$$\langle E_i, D\rangle = z_i^* x x^* z_i = |z_i^* x|^2.$$

This is consistent with our earlier description. The simplest POVM is formed from the matrices $e_i e_i^T$, and a measurement carried out with this POVM is called a *measurement using the standard basis*. We see that

$$\langle e_i e_i^T, D\rangle = e_i^T D e_i = D_{i,i}.$$

Thus if we measure D using the standard basis, the probability we observe outcome i is $D_{i,i}$.

A state in a composite system with r parts will be a convex combination of matrices of the form

$$D_1 \otimes \cdots \otimes D_r,$$

where $D_1, \ldots, D_r$ are density matrices.

If, at time zero, a closed quantum system is in state given by a density matrix D, its state at time t is

$$UDU^*$$

for a unitary matrix U; it is easy to verify that UDU^* is a density matrix. If D is a pure state, say $D = zz^*$, then

$$UDU^* = Uzz^*U^* = Uz(Uz)^*.$$

This is consistent with out earlier description and, as there, typically there is a Hermitian matrix H such that

$$U(t) = \exp(itH).$$

2.3 Qubits and 2×2 Hermitian Matrices

The qubit is the fundamental unit of quantum information—it is the smallest quantum system that could assume more than one single state. It also serves as a building block for larger systems, via the composition operation described earlier. In this sense, it is quite convenient to have a good understanding of what can be done to a qubit, and perhaps even a geometric intuition.

As we have seen, states of qubits correspond are represented by positive semidefinite matrices of trace one. These can be quite conveniently parametrized as we show below.

Let $\mathcal{H}$ denote the real vector space of 2×2 Hermitian matrices. We define an isomorphism Ψ from $\mathbb{R}^4$ to $\mathcal{H}$ by as follows. If

$$v = \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix},$$

then

$$\Psi(v) = \begin{pmatrix} w+z & x-\mathrm{i}y \\ x+\mathrm{i}y & w-z \end{pmatrix}.$$

Together with the identity, the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the images of the standard basis of $\mathbb{R}^4$, and thus

$$\Psi(v) = wI + x\sigma_x + y\sigma_y + z\sigma_z.$$

If we take linear combinations of these matrices, we see that they form a convenient basis for the space of 2×2 Hermitian matrices, orthogonal relative to our inner product on matrices. They are also unitary, and so by taking products and powers only, they generate a subgroup of the group of 2×2 unitary matrices. We see that σ_x and σ_y generate a dihedral group and, as $(\sigma_x\sigma_y)^2 = -I$, this group has order eight. Hence the group generated by the three Pauli matrices has order 16; naturally enough it is known as the Pauli group. Any two Pauli matrices either commute or anticommute—for example, $\sigma_z\sigma_x = -\sigma_x\sigma_z$.

If $H = \Psi(v)$, we find that $\mathrm{tr}(H) = 2\langle e_1, v\rangle = 2w$.

2.3.1 Lemma. *If H is a 2×2 Hermitian matrix, then it is positive semidefinite if and only if* $\operatorname{tr}(H) \geq 0$ *and* $\det(H) \geq 0$.

Proof. If H is a 2×2 positive semidefinite matrix, its eigenvalues are non-negative and so both $\operatorname{tr}(H)$ and $\det(H)$ are non-negative. For the converse, using the above parameterization we see that if $\operatorname{tr}(H) \geq 0$ then $w \geq 0$. As

$$\det(H) = w^2 - x^2 - y^2 - z^2$$

it follows that if $\det(H) \geq 0$, then $w^2 \geq z^2$ and so the diagonal entries of H are non-negative. Therefore both the diagonal entries and determinant of H are non-negative, and hence it is positive semidefinite. □

The Hermitian matrices with rank and trace equal to 1 correspond to the elements of $\mathbb{R}^4$ with $w = 1/2$ and

$$x^2 + y^2 + z^2 = \frac{1}{4}.$$

Thus they correspond to the points on a sphere in $\mathbb{R}^3$, known to physicists as the Bloch sphere. Density matrices, that is, positive semidefinite Hermitian matrices with trace 1, correspond to the points on or inside this sphere.

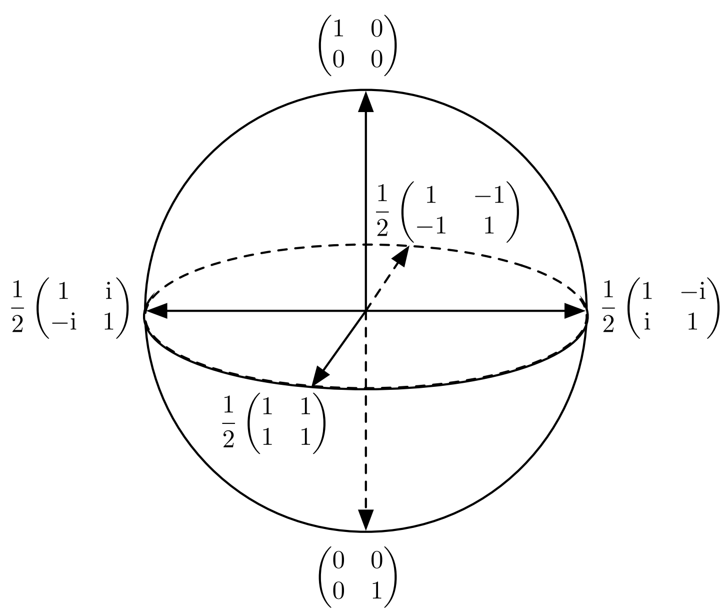

Figure 2.1: The Bloch Sphere and the density matrices corresponding to six points. The origin corresponds to $(1/2)I$.

2.4 Entanglement

Consider quantum systems $\mathbb{C}^k$ and $\mathbb{C}^m$, and their composition given by $\mathbb{C}^k \otimes \mathbb{C}^m \cong \mathbb{C}^{km}$. A density matrix S of dimension $km \times km$ represents a quantum state in the composed system. Even if it has rank 1, therefore corresponding to a pure state, it could be that there are no choices of P and Q, density matrices of dimensions k and m respectively, so that $P \otimes Q = S$. In this case, we say that the state given by S is an *entangled state*. For example, the state on $\mathbb{C}^2 \otimes \mathbb{C}^2$ given by

$$S = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is entangled.

Entanglement can be created (or destroyed) by unitary maps. For instance, if

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix},$$

then

$$USU^* = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

The effect of measurements on entangled states plays an important role in the understanding of quantum mechanics. Using the example above, assume we proceed by measuring the first system according to the observable σ_z, and do nothing in the second, which corresponds to measuring according to I. The measurement in the composed system is given by the observable $\sigma_z \otimes I$. The result of the this measurement is either $+1$ or -1, either with probability $1/2$, and the resulting state of the composed system will be, respectively,

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \text{ or } \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Now, a measurement is performed in the second system according to the same observable σ_z. The result will have complete correlation with the result of the previous measurement in the first system, namely, if the first measurement returns $+1$, the second will return -1, and if the first returns -1, the second will give $+1$.

Returning to the more general setting, say S is a density matrix representing a state in $\mathcal{A} \otimes \mathcal{B} \cong \mathbb{C}^{km}$, written as

$$S = \sum_j P_j \otimes Q_j.$$

Say M is an observable on the first system, with spectral decomposition $M = \sum_r \lambda_r F_r$. Upon measuring the system with respect to an observable $M \otimes I$, we have that the probability of receiving λ_r is given by $\sum_j \langle F_r, P_j \rangle \langle I, Q_j \rangle$. This motivates the definition of the *partial trace* operation. In this case, we are tracing out the second system, receiving

$$\operatorname{tr}_{\mathcal{B}} S = \sum_j (\operatorname{tr} Q_j) P_j.$$

This resulting state is a reduced state in system $\mathcal{A}$, which exhibits the observable quantities of $\mathcal{A}$ in the composed system.

2.5 Walks: Adjacency Matrix

We discuss the physics underlying quantum walks on graphs. If X is a graph on n vertices, then to implement a continuous walk on X we require n qubits. The state space is $(\mathbb{C}^2)^{\otimes n}$. To enable us to describe operations on this space, we choose a basis.

First, let $\{f_0, f_1\}$ denote the standard basis for $\mathbb{C}^2$. Next, if $S \subseteq \{1, \dots, n\}$, we define

$$f_S = f_{i_1} \otimes \cdots \otimes f_{i_n},$$

with $i_r = 1$ if $r \in S$ and $i_r = 0$ otherwise. If $|S| = k$, the vectors f_T such that $T \subseteq S$ span a subspace of the state space with dimension 2^k. The *weight* of the vector f_S is $|S|$. The span of the vectors of weight k is known as the *k-excitation subspace*.

Recall the definition of Pauli matrices σ_x, σ_y and σ_z. If $w \in \{x, y, z\}$, then $\sigma_{w,r}$ denotes the operator on the state space formed by the tensor product of n operators on $\mathbb{C}^2$, where the r-th operator is σ_w and the rest are all equal to the 2×2 identity. We note that any two operators of the form $\sigma_{w,a}\sigma_{w,b}$ (for w in $\{x, y, z\}$ and a, b in $V(X)$) commute. (Exercise.)

We define the *edge-Hamiltonian* $H_{xy}(ab)$ by

$$H_{xy}(ab) = \frac{1}{2}(\sigma_{x,a}\sigma_{x,b} + \sigma_{y,a}\sigma_{y,b}).$$

We see that

$$\sigma_x f_0 = f_1,\ \sigma_x f_1 = f_0$$

and

$$\sigma_y f_0 = \mathrm{i} f_1,\ \sigma_y f_1 = -\mathrm{i} f_0.$$

Accordingly, if $S \oplus T$ denotes symmetric difference of subsets, we have

$$\sigma_{x,a}\sigma_{x,b} f_S = f_{S\oplus\{a,b\}}$$

while

$$\sigma_{y,a}\sigma_{y,b} f_S = -(-1)^{|S\cap\{a,b\}|} f_{S\oplus\{a,b\}}.$$

If follows that

$$\begin{aligned} H_{xy}(ab) f_S &= \frac{1}{2}\Big(1-(-1)^{|S\cap\{a,b\}|}\Big) f_{S\oplus\{a,b\}} \\ &= \begin{cases} f_{S\oplus\{a,b\}}, & |S\cap\{a,b\}| = 1; \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

One consequence of this is that $H_{xy}(ab)$ maps the k-excitation subspace to itself.

Finally, the *xy-Hamiltonian* associated with the graph X is the sum of the edge-Hamiltonians:s

$$H_{xy} := \frac{1}{2}\sum_{ab\in E(X)} (\sigma_{x,a}\sigma_{x,b} + \sigma_{y,a}\sigma_{y,b}).$$

We see at once that the k-excitation subspace is invariant under the action H_{xy} too. Let W_k denote the k-excitation subspace If the initial state of quantum system evolving under the unitary transition matrix

$$U(t) = \exp(\mathrm{i}tH_{xy})$$

lies in W_k then, for any time t, the state of the system lies in W_k. The matrix that represents the action of H_{xy} to W_1 is the adjacency matrix A

of X. The quantum system that arises by restriction to W_1 is the continous quantum walk on X; its transition matrix is $\exp(itA)$.

For each space W_k is invariant under the Hamiltonian H_{xy}, and there is an interesting combinatorial description of the matrix representing the restriction of H_{xy} to W_k. We have just seen that it is the adjacency matrix of X when $k = 1$.

The *k-th symmetric power* $X^{\{k\}}$ of a graph X has the k-subsets of $V(X)$ as vertices, where two k-subsets are adjacent if their symmetric difference is an edge of X. Note that $X^{\{1\}} \cong X$ and, if $X = K_n$, then $X^{\{2\}}$ is isomorphic to the line graph $L(K_n)$. We also see (more precisely, you may verify) that $X^{\{n-k\}} \cong X^{\{k\}}$.

2.5.1 Theorem. *The matrix that represents the action of H_{xy} on the span of the vectors f_S where $|S| = k$ is the adjacency matrix of the k-th symmetric power of the graph X.*

Proof. We have

$$H_{xy} f_S = \sum_{ab \in E(X)} H_{xy}(ab) f_S = \sum_{T : S \oplus T \in E(X)} f_T.$$

As the last sum is over the neighbours of S in $X^{\{k\}}$, we are done. □

2.6 Walks: More Matrices

We have seen that the edge-Hamiltonian $H_{xy}(ab)$ leads to quantum walks based on the adjacency matrix of a graph. There are other forms of adjacency matrix of graphs, and some of this give rise to continuous walks.

Let X be a graph on n vertices with adjacency matrix A and let Δ be the diagonal matrix of order $n \times n$ with $\Delta_{i,i}$ equal to the valency of the i-th vertex of x. The *Laplacian matrix* $L(X)$ is defined by

$$L(X) = \Delta - A.$$

The *unsigned Laplacian* of X is the matrix

$$\Delta + A;$$

it does not have a standard symbol and has received much less attention than the Laplacian. Both forms of Laplacian are positive semidefinite.

We define an edge-Hamiltonian by

$$H_{xyz}(ab) = \frac{1}{2}(\sigma_{x,a}\sigma_{x,b} + \sigma_{y,a}\sigma_{y,b} + \sigma_{z,a}\sigma_{z,b})$$

and observe that (we observe, you prove)

$$H_{xyz}(ab)f_S = \frac{1}{2}\Big(1 - (-1)^{|S\cap\{a,b\}|}\Big)f_{S\oplus\{a,b\}} + \frac{1}{2}(-1)^{|S\cap\{a,b\}|}f_S$$

The subspaces W_k are invariant under this operator, and so they are also invariant under the *xyz-Hamiltonian* or Heisenberg Hamiltonian is

$$H_{xyz} = \frac{1}{2}\sum_{ab\in E(X)}(\sigma_{x,a}\sigma_{x,b} + \sigma_{y,a}\sigma_{y,b} + \sigma_{z,a}\sigma_{z,b}).$$

If $\Delta(X^{\{k\}})$ is the diagonal matrix that records the degrees of the vertices in $X^{\{k\}}$, then on W_k, the operator H_{xyz} is represented by the matrix

$$\frac{1}{2}|E(X)|I + A(X^{\{k\}}) - \Delta(X^{\{k\}}),$$

When $k = 1$, this is essentially the Laplacian matrix of X.

We can also realize the so-called unsigned Laplacian—for the Hamiltonian

$$H_{xy\bar{z}} = \frac{1}{2}\sum_{ab\in E(X)}(\sigma_{x,a}\sigma_{x,b} + \sigma_{y,a}\sigma_{y,b} - \sigma_{z,a}\sigma_{z,b}),$$

the representing matrix is

$$-\frac{1}{2}|E(X)|I + A(X^{\{k\}}) + \Delta(X^{\{k\}}).$$

When the underlying graph X is regular, Δ is a scalar matrix and the adjacency matrix and the two Laplacians provide the same information. It seems the perfect state transfer occurs less frequently when we use the Laplacian in place of the adjacency matrix. Nothing is known about the unsigned Laplacian.

2.7 Orbits of Density Matrices

Assume A is the adjacency matrix of X on n vertices and $U(t) = \exp(\mathrm{i}tA)$. Then the set

$$\mathcal{U} := \{t \in \mathbb{R} : U(t)\}$$

is a group. It is in fact the image of a homomorphism from the additive group $\mathbb{R}$ into the group $U(n)$ of $n \times n$ unitary matrices; it is a so-called *1-parameter subgroup* of $U(d)$. Since $\mathbb{R}$ is abelian, $\mathcal{U}$ is abelian.

The group $\mathcal{U}$ acts on the set of $n \times n$ density matrices:

$$D \mapsto U(t)DU(-t).$$

We use $D(t)$ to denote $U(t)DU(-t)$. The set $\{D(t) : t \in \mathbb{R}\}$ is the orbit of D under this action of $\mathcal{U}$. Our concern is with *forward orbits*, that is, sets of the form

$$\{D(t) : t \geq 0\}.$$

If $a, b \in V(X)$, it follows that we have perfect state transfer (as defined in Section 1.3)from a to b if and only if D_b lies in the orbit of D_b. Further, if D_b lies in the orbit of D_a, then the orbits of D_a and D_b are equal, implying that if there is perfect state transfer for a to b, we must also perfect state transfer from b to a. This viewpoint provides a geometric interpretation of perfect state transfer.

The orbit of D is a curve in the set of density matrices. One thing to note is that points on this curve do not always form a closed set. To see this, recall that the path P_4 admits pretty good state transfer between its end-vertices 1 and 4. Now you can show that there is perfect state transfer from a to b if and only if D_b lies in the closure of the orbit of D_a. Since we do **not** have perfect state transfer from 1 to 4 in P_4, the closure of the orbit of D_1 contains a point not on the orbit.

If D_b lies in the closure of the orbit of D_a, then the orbit of D_b lies in the closure of the orbit of D_a, whence we see that if there is pretty good state transfer from a to b, there must be pretty good state transfer from b to a.

2.7.1 Lemma. *The closure of the orbit of a matrix D under $\mathcal{U}$ is equal to the orbit of D under the closure of $\mathcal{U}$.*

Proof. There are two parts. First show that the orbit of D under $\overline{\mathcal{U}}$ is closed. Then show that if $M \in \overline{\mathcal{U}}$ and M is close to $U(t)$ for some t, then

MDM^* is close to a point in the orbit of D under $\mathcal{U}$. (Detils left to the reader.) □

We have seen that a continuous quantum walk on particular graph may be periodic, i.e., there is a time τ such that $U(n\tau) = I$ for all integers n. We show that any continuous quantum walk is, in a sense, approximately periodic.

2.7.2 Theorem. *Let $U(t)$ be the transition matrix of the continuous quantum walk on the graph X. For any $\tau > 0$ and any $\epsilon > 0$, there is a positive integer k such that $\|U(k\tau) - I\| < \epsilon$.*

Proof. Assume $n = |V(X)|$ and consider the sequence $U(m\tau)$. It is infinite but lies in the compact group $U(n)$, and consequently it has a limit point M in $U(n)$. Hence there are distinct integers ℓ and m such that

$$\|U(\ell\tau) - M\| < \epsilon/2, \quad \|U(m\tau) - M\| < \epsilon/2.$$

By the triangle inequality we then have

$$\|U(m\tau) - U(\ell\tau)\| < \epsilon$$

and, since $U(t)$ is unitary

$$\|U(m\tau) - U(\ell\tau)\| = \|U(\ell\tau)(U((m-\ell)\tau) - I)\| = \|U((m-\ell)\tau) - I\|.$$

Take $k = m - \ell$ to get the theorem. □

This theorem tells us that a quantum walk returns 'close' to its initial state infinitely often. We will revisit this topic in Chapter 8.

Notes

We list some of the books that we have found useful in our attempts to get a better handle on the physics side of things. And to help the reader calibrate our weightings, note that (when reading) we prefer thin books to fat ones, and that we are not particularly concerned with algorithmic questions.

Quantum Computing, Quantum Information Theory

(a) Barnett, “Quantum Information” [6].

(b) Kaye, Laflamme, Mosca, “An Introduction to Quantum Computing”.

(c) Mermin, “Quantum Computer Science: An Introduction” [47].

(d) Nielsen and Chuang, “Quantum Computation and Quantum Information” [49].

(e) Petz, “Quantum Information Theory and Quantum Statistics” [51].

(f) Watrous, “The Theory of Quantum Information" [59].

Quantum Physics

(a) Schumacher and Westmoreland, “Quantum Processes, Systems & Information” [53]. An introduction designed for quantum computing.

(b) Brian C. Hall, “Quantum Theory for Mathematicians” [40].

(c) Shlomo Sternberg, “A Mathematical Companion to Quantum Mechanics” [**?**].

(d) Gerald Teschl, “Mathematical Methods in Quantum Mechanics” [55].

Lie Groups

(In decreasing order of sophistication.)

(a) Daniel Bump, “Lie Groups” [].

(b) Brian C. Hall, “Lie Groups, Lie Algebras, and Representations” [].

(c) John Stillwell, “Naive Lie Theory” [].

Exercises

2-1. Verify that if w in $\{x, y, z\}$ and a, b in $V(X)$, then any two operators of the form $\sigma_{w,a}\sigma_{w,b}$ commute.

2-2. Compute the matrix H_{xy} explicitly for the graph P_3. Identify its blocks, and realize what their column and row indices mean.

2-3. Assume a system of n qubits is put under the action of the xy-Hamiltonian. Show that if the initial state of each qubits is f_0, then nothing happens.

2-4. Show that if P_1, P_2 and P_3 are orthogonal projections, and that $I = \sum_{i=1}^{3} P_i$, then $P_i P_j = 0$ for all $i \neq j$. As a challenge, extend this result to k projectors instead of only three.

2-5. Show that if D_b lies in the closure of the orbit of D_a, then the orbit of D_b lies in the closure of the orbit of D_a. Using this, deduce that if we have pretty good state transfer from a to b, there is also pretty good state transfer from b to a.

Part II

Spectra of Graphs

Chapter 3

Equitable Partitions

We develop some of the theory of equitable partitions. As we will see, sometimes it is possible to partition the vertex set of a graph in such a way that a quantum walk cannot distinguish between vertices that belong to a class of the partition. This provides a very useful tool to analyse certain quantum phenomena in graphs.

The concept of equitable partitions in algebraic graph theory has been used for some time. There are treatments of this topic in [35, 38], and the reader who finds the treatment here too terse may find these sources useful.

3.1 Partitions and Projections

If π is a partition, then $|\pi|$ denotes the number of cells of π. We want to represent partitions by matrices, as follows. If π is a partition of $V(X)$, its *characteristic matrix* S is the matrix whose columns are the characteristic vectors of the cells of π, that is, each column is a 01-vector that records in each row whether a vertex belongs to the cell. The column space of S is precisely the space of real functions on $V(X)$ that are constant on the cells of π. Sometimes we will need the *normalized characteristic matrix*, which get by scaling each column so that it has norm 1. We denote this matrix by $\widehat{S}$ and observe that

$$\widehat{S}^T\widehat{S} = I_{|\pi|}.$$

Note that S and $\widehat{S}$ have the same column space. Since $\widehat{S}\widehat{S}^T$ is idempotent, it follows it is the matrix that represents orthogonal projection onto the space of functions constant on the cells of π.

A partition $\pi = (C_1, \ldots, C_k)$ of $V(X)$ is *equitable* if the number of neighbours in C_j of a vertex in C_i is the same for all vertices in C_i (including the case $i = j$).

Given an equitable partition π of X, we define the *quotient graph* X/π to be the directed graph with the cells of π as its vertices, and with the number of arcs from the cell C_i to the cell C_j equal to the number of neighbours in C_j of a vertex in C_i. If $B = A(X/\pi)$ is the adjacency matrix of this directed graph, note that $AS = SB$.

For example, any partition of the vertex set of C_4 into two parts of size two provides an equitable partition. You are invited to determine all possible equitable partitions of P_3, P_4 and C_5.

The fundamental characterizations of equitable partitions are given by the following.

3.1.1 Lemma. *Let π be a partition of $V(X)$ with characteristic matrix S and normalized characteristic matrix $\widehat{S}$. The following are equivalent:*

(a) π is equitable.

(b) $\mathrm{col}(S)$ is A-invariant.

(c) A and $\widehat{S}\widehat{S}^T$ commute.

Proof. The definition of equitable partition implies that π is equitable if and only if there is a matrix B such that $AS = SB$, and this is equivalent to requiring that $\mathrm{col}(S)$ is A-invariant. Hence (a) and (b) are equivalent.

Since $\mathrm{col}(S) = \mathrm{col}(\widehat{S})$ we see that if π is equitable then $A\widehat{S} = \widehat{S}C$ for some matrix C and then

$$A\widehat{S}\widehat{S}^T = \widehat{S}C\widehat{S}^T.$$

As $A\widehat{S} = \widehat{S}C$ we have $C = \widehat{S}^T A\widehat{S}$, from which we see that C is symmetric. We have

$$\widehat{S}\widehat{S}^T A = \widehat{S}(A\widehat{S})^T = \widehat{S}(\widehat{S}C)^T = \widehat{S}C\widehat{S}^T$$

and so (b) implies (c).

To prove that (c) implies (b), we observe that, as a consequence of (c), $A\widehat{S} = \widehat{S}\widehat{S}^T A\widehat{S}$, thus $\mathrm{col}(\widehat{S})$ is A-invariant. □

The equivalence of (b) and (c) is purely a fact from linear algebra: if A is symmetric, then a subspace U is A-invariant if and only if the matrix representing orthogonal projection on U commutes with A.

The matrix $\widehat{S}\widehat{S}^T$ is doubly stochastic and represents orthogonal projection onto the space of functions constant on the cells of π. It is a block diagonal matrix with diagonal blocks $\frac{1}{r}J_r$, where J_r is the all-ones matrix of order $r \times r$, and the size of the i-th block is the size of the i-th cell of π. The vertex u forms a singleton cell of π if and only if $\widehat{S}\widehat{S}^T e_u = e_u$.

We view $C = \widehat{S}^T A \widehat{S}$ as the adjacency matrix of the *symmetrized quotient graph* of X relative to π. Note that C is diagonally similar to $A(X/\pi)$. We can compute its spectral decomposition as follows. Since A is symmetric, it has a spectral decomposition

$$A = \sum_{r=0}^{d} \theta_r E_r$$

where θ_r runs over the distinct eigenvalues θ_r of A and E_r is the matrix that represents orthogonal projection onto the the eigenspace belonging to θ_r.

3.1.2 Lemma. *Let π be an equitable partition of X with normalized characteristic matrix $\widehat{S}$. Let A be the adjacency matrix of X and let C be the adjacency matrix of the symmetrized quotient graph, that is, $C = \widehat{S}^T A \widehat{S}$. Then the idempotents in the spectral decomposition of C are the non-zero matrices $\widehat{S}^T E_r \widehat{S}$, where E_r runs over the idempotents in the spectral decomposition of A.*

Proof. From

$$A = \sum_{r=0}^{d} \theta_r E_r,$$

we have

$$C = \widehat{S}^T A \widehat{S} = \sum_{r=0}^{d} \theta_r \widehat{S}^T E_r \widehat{S}. \tag{3.1.1}$$

Note that $\widehat{S}^T E_r \widehat{S}$ is symmetric. As π is equitable, $\widehat{S}^T \widehat{S}$ commutes with A, thus commutes with all E_r, which are polynomials in A. Hence

$$(\widehat{S}^T E_r \widehat{S})(\widehat{S}^T E_s \widehat{S}) = \widehat{S}^T E_r E_s \widehat{S},$$

thus the $\widehat{S}^T E_r \widehat{S}$ are orthogonal idempotents. Finally,

$$\sum_{r=0}^{d} \widehat{S}^T E_r \widehat{S} = \widehat{S}^T \widehat{S} = I,$$

thus we conclude that (3.1.1) is the spectral decomposition of C. □

Note the corresponding idempotents are associated to the same eigenvalues.

3.2 Walks and Orthogonal Matrices

With just the characterization of the previous section in hand, we have some useful consequences.

3.2.1 Lemma. *Suppose π is an equitable partition of X and that a cell of π is a singleton containing the vertex a, call it $\widehat{a} = \{a\}$. Let C be the adjacency matrix of the symmetrized quotient graph relative to π. Let $b \in V(X)$, and $\widehat{b}$ the class of π containing b. Then, for any time t:*

(a) $U(t)e_a$ is constant on the cells of π.

(b) $U(t)_{a,b} = (1/\sqrt{|\widehat{b}|})(\exp \mathrm{i}tC)_{\widehat{a},\widehat{b}}$.

Proof. To see (a), let S be the characteristic matrix of π. Because $\{a\}$ is a cell, we have

$$U(t)e_a = U(t)Se_a.$$

As the column space of S is A invariant, it is also $U(t)$ invariant, so any column of $U(t)S$ is constant in the cells of π. In particular, $U(t)e_a$ is constant in the cells of π.

To see (b), it suffices to note that, as $\widehat{S}\widehat{S}^T$ commutes with A, we have

$$\widehat{S}^T \exp(\mathrm{i}tA)\widehat{S} = \exp(\mathrm{i}t\widehat{S}^T A\widehat{S}) = \exp(\mathrm{i}tC),$$

and then apply (i). □

Item (b) immediately gives the corollary below.

3.2.2 Corollary. *Assume there exists an equitable partition in X in which $\{a\}$ is a cell. We have perfect state transfer on X from a to b at time t if and only if the symmetrized quotient graph has perfect state transfer from $\{a\}$ to $\widehat{b}$, and in this case, $\widehat{b} = \{b\}$.*

We actually can say something a bit stronger. If D is a pure state, then $D^2 = D$ and consequently if D_1 and D_2 are pure states,

$$\|D_1 - D_2\|^2 = \mathrm{tr}(D_1 - D_2)^2 = \mathrm{tr}(D_1 + D_2 - 2D_1D_2) = 2 - 2\langle D_1, D_2\rangle.$$

Thus $D_1 = yy^*$ and $D_2 = zz^*$, this yields that $\|D_1 - D_2\|^2 = 2 - 2|y^* z|^2$.

Recall the abbreviated notation $D_a(t) = U(t) D_a U(-t)$.

3.2.3 Lemma. *Assume P is an orthogonal matrix that commutes with $A(X)$, with $Pe_a = e_a$. Then*

$$\|D_b - PD_bP^T\| \leq 2\|D_a(t) - D_b\|.$$

Proof. We have

$$\begin{aligned} P(D_a(t) - D_b)P^T &= PU(t)D_aU(-t)P^T - PD_bP^T \\ &= U(t)PD_aP^TU(-t) - PD_bP^T \\ &= U(t)D_aU(-t) - PD_bP^T \\ &= D_a(t) - PD_bP^T. \end{aligned}$$

As P is orthogonal, this implies that

$$\|D_a(t) - D_b\| = \|D_a(t) - PD_bP^T\|$$

and hence if $\|D_a(t) - D_b\| = \delta$, then by the triangle inequality,

$$\|D_b - PD_bP^T\| \leq 2\delta.$$

□

3.2.4 Lemma. *Suppose $a, b \in V(X)$, and $|V(X)| = n$. If $\|D_a(t) - D_b(t)\| < 1/\sqrt{n}$ for some t, then any equitable partition in which $\{a\}$ is a singleton cell must also have $\{b\}$ as a singleton cell.*

Proof. Suppose that we have an equitable partition π in which $\{u\}$ is a singleton cell, and let $M = \widehat{S}\widehat{S}^T$ represent orthogonal projection onto the space of functions constant on the cells of π. Let $P = 2M - I$. This is an orthogonal matrix (verify it as an exercise), commutes with A (due to Lemma 3.1.1) and $Pe_a = e_a$ (as $\{a\}$ is a cell). We can apply the lemma, giving

$$\|D_b - PD_bP^T\| \leq 2||D_a(t) - D_b|| < 2/\sqrt{n}.$$

Now if b lies in a cell of π with size k, then

$$\|D_b - PD_bP^T\|^2 = 2 - 2\langle D_b, PD_bP^T\rangle = 2 - 2\left(\frac{2}{k} - 1\right)^2 = \frac{8}{k}\left(1 - \frac{1}{k}\right).$$

If $k = 1$ this is equal to 0, and we are in good terms. Otherwise, $2 \leq k \leq n$. In this case,

$$\frac{8}{k}\left(1 - \frac{1}{k}\right) \geq \frac{4}{k} \geq \frac{4}{n},$$

a contradiction. □

3.3 Automorphisms

Recall that an *automorphism* of a graph X is a bijection $f : V(X) \to V(X)$ that maps edges to edges, that is, $a \sim b$ if and only if $f(a) \sim f(b)$. The set of all automorphisms of a graph forms a group called the automorphism group of X, or $\mathrm{Aut}(X)$. To each permutation f of the vertices of X, there is a corresponding permutation matrix P. It is easy to verify that f is an automorphism if and only if P and A commute.

The *orbit of a vertex* $a \in V(X)$ is the subset of X determined by

$$a^{\mathrm{Aut}(X)} = \{b \in V(X) : f(a) = b \text{ for some } f \in \mathrm{Aut}(X)\}.$$

It is a standard exercise to verify that the orbits of $\mathrm{Aut}(X)$ partition $V(X)$; we call this the *orbit partition*. It is actually more interesting to verify that this partition is equitable.

3.3.1 Lemma. *If $G \leq \mathrm{Aut}(X)$, the orbit partition relative to G is equitable.*

Proof. If A is the adjacency matrix, S is the characteristic matrix of the partition and P is the permutation matrix of an automorphism, note that first that $PS = S$. Then

$$AS = APS = PAS.$$

So the columns of AS are invariant under P. But this is true for all automorphisms, thus the columns of AS are constant in each orbit. Therefore the column space of S is A-invariant, and the result follows from Lemma 3.1.1. □

If Q is a permutation matrix with multiplicative order k then

$$C = \frac{1}{k}(I + Q + \cdots + Q^{k-1})$$

is doubly stochastic and represents orthogonal projection onto the functions constant on the orbits of Q. If M represents orthogonal projection onto the space of functions constant on the cells of a partition π of $V(X)$ and $a \in V(X)$, then $Me_a = e_a$ if and only if $\{a\}$ is a cell of π. So $Ce_a = e_a$ if and only if a is fixed by the automorphism Q.

If G is a permutation group acting on a set V and $a \in V$, we use G_a to denote the *stabilizer* of a in G, that is, the subgroup formed by the permutations in G that fix a. The previous results applied to the orbit partition of $\mathrm{Aut}(X)_a$ yields:

3.3.2 Corollary. *Let G be the automorphism group of X. If we have perfect state transfer from a to b, then $G_a = G_b$.*

Proof. The group G_a is a subgroup of $\mathrm{Aut}(X)$. The orbit of a contains only itself, thus $\{a\}$ is a singleton of an equitable partition of $V(X)$. By Corollary 3.2.2, $\{b\}$ is also a singleton, so any automorphism fixing a also fixes b. As we shall also have state transfer from b to a, it follows that $G_a = G_b$. □

Again, we can say something stronger by applying Lemma 3.2.3, noting that a permutation matrix is an orthogonal matrix.

3.3.3 Lemma. *Let a and b be vertices of X. If there is a time t such that $\|D_a(t) - D_b\| < 1/\sqrt{2}$, then any automorphism of X that fixes a must also fix b.*

Proof. Assume P is the matrix corresponding to an automorphism, and $Pe_a = e_a$. From Lemma 3.2.3, we have

$$\|D_b - PD_bP^T\| < \sqrt{2}.$$

If $Pe_b = e_c$ for some vertex c, we have $PD_bP^T = D_c$. If $b \neq c$, then

$$\|D_b - PD_bP^T\|^2 = \|D_b - D_c\|^2 = 2.$$

We conclude that if there is a time t such that $\|D_a(t) - D_b(t)\| < 1/\sqrt{2}$, then any automorphism of X that fixes a must also fix b. □

A physicist would say that a unitary matrix that commutes with A is a symmetry of the quantum system determined by A. Both automorphisms and equitable partitions give rise to symmetries in this sense (but there will be many symmetries that do not arise in this way). We will meet some of them in Section 7.2, and we shall prove further results that resemble some of the above.

3.4 Quotients of the d-Cube and of Complete Bipartite Graphs

Lemma 3.2.1 has shown that in the presence of an equitable partition that singles out a vertex in a cell, any question about the quantum walk that starts on this vertex of the graph can be reduced to a question about a quantum walk on a smaller, albeit weighted, graph. In this section, we display an application to the d-cube. One way to define the d-cube is to say that vertices are the $\{0,1\}$ strings of length d, with adjacency if and only if two strings differ in one position.

Let π denote the distance partition relative to a vertex a in the d-cube Q_d. This means that $\{a\}$ is a singleton, and each of the other classes of the partition correspond to vertices at a fixed distance from a. We can assume that a is the all 0s string, and it is not so difficult now to convince yourself that the vertices at distance k from $\{a\}$ are precisely those with k entries equal to 1. Further, and we leave this as an exercise, this distance partition is equitable. In fact, all distance partitions of vertices of the d-cube are equitable, and the quotient graphs are all equal. The quotient graph of a distance partition of the d-cube is a weighted path with $d+1$ vertices, and no loops.

If $B = A(Q_d/\pi)$ is the adjacency matrix of this quotient, then $B_{r,s} = 0$ if $|r-s| \neq 1$, that is, $A(Q_d/\pi)$ is a weighted path with no loops, and

$$B_{r,s} = \begin{cases} d-r, & r = s-1, \\ r, & r = s+1. \end{cases}$$

From Lemma 3.2.1, we have

$$U_B(t)_{\{u\},\{v\}} = U(t)_{u,v}.$$

Since we have perfect state transfer on the d-cube between u and v at time $\pi/2$ (recall Chapter 1), it follows that we have perfect state transfer on our weighted path at time $\pi/2$.

This has the important consequence that, if we can use weights and directions in edges, we can always arrange for perfect state transfer at arbitrary distances in paths. We shall return to this topic in depth in Chapter 13.

As a second application of these ideas, we consider the quantum walk on the complete bipartite graphs $K_{2,n}$. Denote the two vertices of the degree n by a and b. Then the sets

$$\{a\},\ \{b\},\ V(X)\setminus\{a,b\}$$

are the cells of an equitable partition, and the adjacency matrix of the symmetrized quotient is

$$\begin{pmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & 0 & \sqrt{n} \\ 0 & \sqrt{n} & 0 \end{pmatrix}.$$

But this is just $\sqrt{n}A(P_3)$. We conclude that we have perfect state transfer between a to b at time $\pi/\sqrt{2n}$.

Notes

The first systematic applications of equitable partitions to continuous quantum walks were presented by Ge et al. [30] and Bachman et al. [5].

The material in Section 3.3 is based closely on [31].

In [5], R. Bachman et al. studied perfect state transfer of quantum walks on quotient graphs. They showed that the ab-entry of the transition function $\exp(\mathrm{i}A(X)t)$ of an original graph X is equal to the $\{a\}\{b\}$-entry of the transition function $\exp(\mathrm{i}A(X/\pi)t)$ of the quotient graph with equitable distance partition with respect to vertices a and b. In Lemma 3.2.1, we saw that this is actually an instance of a more general result.

Bachman et al. provided an extensive treatment of some graphs whose quotients are weighted P_4. In particular, by taking two non-isomorphic regular graphs with the same valency and size, constructing two cones over each using distinct vertices a and b, and then creating some edges between the two regular graphs in such a way that the distance partition of a is equitable, they were able to show that if the parameters are right, then there is perfect state transfer between a and b. However there is no automorphism that swaps a and b. This was the first counter-example to the early conjecture that perfect state transfer would imply the existence of an automorphism swapping the vertices involved. We recommend reading this paper for a more hands-on presentation of equitable partitions in the context of quantum walks.

A final philosophical comment. The key to understanding a linear operator is to identify its invariant subspaces, and small invariant subspaces are easier to deal with than large ones. Equitable partitions provide invariant subspaces, however these subspaces have a special property: they have bases of 01-vectors.

Exercises

3-1. Verify that if Q is a symmetric projection matrix, then $(2Q - I)$ is an orthogonal matrix.

3-2. Describe all possible equitable partitions of the graphs P_3, P_4 and C_5.

3-3. Describe all possible equitable partitions of the path P_n. (You might find useful to first show that the $n \times n$ anti-diagonal matrix is a polynomial in $A(P_n)$.)

3-4. Provide a proof for Lemma 3.3.1 that makes no mention to a matrix.

3-5. Show then that the distance partition of any vertex in the d-cube is equitable (it might be useful to start by showing that the d-cube is vertex-transitive, so you only need to consider as the initial vertex the string of 0s). Verify that the weights presented in the text are correct.

3-6. Given a symmetric matrix M, a partition π of its rows (and columns), having characteristic matrix S, will be called equitable if the column space of S is M-invariant. Describe combinatorially what it means for a partition of the vertex set of a graph to be equitable relative to the Laplacian matrix.

Chapter 4

Spectrum and Walks

We investigate expressions for various walk generating functions on a graph X in terms of characteristic polynomials of X and of various induced subgraphs. Although many of the results are known, we offer new proofs in a number of cases. Our motivation, of course, is to relate these concepts to conditions directly related to quantum walk phenomena.

Consider a graph X with vertices a and b. Say $A(X) = \sum_{r=0}^{d} \theta_r E_r$ is the spectral decomposition of A. In Section **??** we saw that if there is perfect state transfer from a to b then a and b were strongly cospectral, that is,

$$E_r e_b = \pm E_r e_a \quad (r = 0, \ldots, d).$$

This implies that a and b are cospectral, one characterization of which is that

$$(A^k)_{a,a} = (A^k)_{b,b}$$

for each k. We have

$$(A^k)_{a,a} = \sum_r \theta_r^k (E_r)_{a,a},$$

indicating a connection between cospectrality and walks, and hence between perfect state transfer and walks. The goal of this chapter is two develop these connnections further.

4.1 Formal Power Series

Given a sequence of elements from a ring $\alpha = (\alpha_k)_{k\geq 0}$, one defines the generating function associated to this sequence with indeterminate t by

$$\alpha(t) = \sum_{k\geq 0} \alpha_k t^k.$$

Typically the the ring is a field, but in the following sections of this chapter it will be a ring of matrices. Despite the perhaps misleading name and notation that suggests $\alpha(t)$ is a function, this power series should be seen as a formal object. The key is that addition and multiplication are well defined operations, and (as we wiol see) under these operations power series for a ring. You should not worry, for example, whether whether the infinite sum converges or not for some non-zero value of the variable. Instead, our only concern is to know or compute or discover or be able to find all coefficients of a power series by a finite process.

(i) Given two power series $\alpha(t) = \sum_{k\geq 0} \alpha_k t^k$ and $\beta(t) = \sum_{k\geq 0} \beta_k t^k$, their sum is defined as:

$$\alpha(t) + \beta(t) = \sum_{k\geq 0} (\alpha_k + \beta_k) t^k.$$

(ii) Given two power series $\alpha(t)$ and $\beta(t)$, their product is defined as:

$$\alpha(t)\beta(t) = \sum_{k\geq 0} \left(\sum_{j=0}^{k} \alpha_j \beta_{k-j} \right) t^k.$$

The set of power series with elements from a ring thus also form a ring. Sometimes, given a power series $\alpha(t)$, it is possible to find its multiplicative inverse, that is, a power series $\beta(t)$ so that $\alpha(t)\beta(t) = 1$. For example, if $\alpha(t) = \sum_{k\geq 0} a^k t^k$, for some a, then $\alpha(t)\beta(t) = 1$ implies that $\beta_0 = 1$, then $\beta_1 = -a$, and the remaining βs equal to 0. Thus,

$$\left(\sum_{k\geq 0} a^k t^k \right) (1 - at) = 1.$$

4.2 Walk Generating Functions

Two graphs are *cospectral* if their adjacency matrices have the same spectrum. We use $\phi(X,t)$ to denote the characteristic polynomial of the adjacency matrix A of X—so $\phi(X,t) = \det(tI - A)$.

We are going to make use of the connection between the spectrum of a graph and various classes of walks. Recall that $(A^k)_{a,b}$ counts the number of walks with k steps from vertex a to vertex b. We will make much use of the *walk generating function*

$$W(X,t) := \sum_{k\geq 0} A^k t^k = (I - tA)^{-1}.$$

One may view a power series whose coefficients are matrices as a matrix whose entries are power series. Thus, the coefficient of t^k in the (a,b) entry of W counts the number of walks with k steps from a to b. Since $\operatorname{tr}(A^k)$ is the number of closed walks of length k in X, it follows that the generating function for closed walks on X (weighted by length) is $\operatorname{tr}(W(X,t))$. From the identity

$$(I - tA)^{-1} = \sum_{r=0}^{d} \frac{1}{1 - t\theta_r} E_r,$$

we have an expression for the generating function for the walks in X that go from u to v:

$$W_{a,b}(X,t) = \sum_{r=0}^{d} \frac{1}{1 - t\theta_r} (E_r)_{a,b}. \tag{4.2.1}$$

4.2.1 Lemma. *Let m_r denote the multiplicity of θ_r as an eigenvalue of X. Then we have the following expression for the generating function for the closed walks on X:*

$$\operatorname{tr}(W(X,t)) = \sum_{r=0}^{d} \frac{m_r}{1 - t\theta_r} = t^{-1} \frac{\phi'(X,t^{-1})}{\phi(X,t^{-1})}$$

Proof. The first equality following from the fact that $\operatorname{tr} E_r = m_r$. For the second equality, we use that

$$\phi(X,t) = \prod_{r=0}^{d} (t - \theta_r)^{m_r},$$

and thus

$$\phi'(X,t) = \sum_{r=0}^{d} m_r (t-\theta_r)^{m_r - 1} \prod_{s\neq r} (t-\theta_s)^{m_r}.$$

Then

$$\frac{\phi'(X,t)}{\phi(X,t)} = \sum_{r=0}^{d} \frac{m_r}{t-\theta_r},$$

and replacing t by $1/t$, we have

$$\frac{\phi'(X,t^{-1})}{\phi(X,t^{-1})} = \sum_{r=0}^{d} \frac{t m_r}{1-t\theta_r}. \qquad \square$$

4.3 Closed Walks at a Vertex

Properties about the determinant that you can prove exploring its Laplace expansion still hold true if the entries of the matrix are power series, in particular, for any matrix M with coefficients which are power series,

$$M \cdot \operatorname{adj}(M) = \det(M) I. \tag{4.3.1}$$

We use $M[j,i]$ to denote the matrix M with row j and column i removed. Then $\operatorname{adj}(M)$ is the matrix defined as

$$(\operatorname{adj} M)_{ij} = (-1)^{i+j} \det M[j,i],$$

Specifically, we are interested in what happens when $M = (I - tA)$. Equation (4.3.1) implies

$$W(X,t) = \frac{\operatorname{adj}(I-tA)}{\det(I-tA)} \tag{4.3.2}$$

If $a \in V(X)$, then $W_{a,a}(X,t)$ is the diagonal entry of $W(X,t)$ corresponding to a, so it follows that

$$W_{a,a}(X,t) = \frac{\det(I - tA(X\setminus a))}{\det(I-tA)},$$

which we prefer to write as

$$t^{-1} W_{a,a}(X,t^{-1}) = \frac{\phi(X\setminus a, t)}{\phi(X,t)}. \tag{4.3.3}$$

On the other hand

$$t^{-1}W(X,t^{-1}) = \sum_{r=0}^{d} \frac{1}{t-\theta_r} E_r,$$

thus

$$\frac{\phi(X \setminus a, t)}{\phi(X,t)} = \sum_{r=0}^{d} \frac{(E_r)_{a,a}}{t-\theta_r}. \tag{4.3.4}$$

As a consequence, and using Lemma 4.2.1,

4.3.1 Corollary. *For any graph X we have*

$$\phi'(X,t) = \sum_{a \in V(X)} \phi(X \setminus a, t). \qquad \square$$

Suppose $a \in V(X)$ and $b \in V(Y)$. We say that the pairs (X,a) and (Y,b) are *cospectral* if X is cospectral to Y and $X\backslash a$ is cospectral to $Y\backslash b$. If $X = Y$, then (X,a) is cospectral do (X,b) if and only if $\phi(X \setminus a, t) = \phi(X \setminus b, t)$, in which case we may simply say that a and b are cospectral. This definition, of course, is equivalent to the one we presented in the beginning of this chapter.

4.3.2 Theorem. *Given X and $A(X) = \sum_{r=0}^{d} \theta_r E_r$, and vertices a and b, the following are equivalent:*

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

(b) $(E_r)_{a,a} = (E_r)_{b,b}$ *for all r.*

(c) $(A^k)_{a,a} = (A^k)_{b,b}$ *for all integers k.*

(d) $W_{a,a}(X,t) = W_{b,b}(X,t)$.

Proof. From Equation (4.3.4), it follows that

$$(E_r)_{a,a} = \left.\frac{\phi(X \setminus a, t)(t-\theta_r)}{\phi(X,t)}\right|_{t=\theta_r}.$$

Thus (a) gives (b). Conditions (b) and (c) are equivalent because A^k is a linear combination of $E_0, \ldots, E_d$, and each E_r is a polynomial in A. From (b) to (d), it follows immediately from Equation (4.2.1). From (d) to (a), we use Equation (4.3.3). $\square$

4.3.3 Corollary. *If there is perfect state transfer between two vertices, then they have the same valency.*

Proof. As we have seen, vertices involved in perfect state transfer are cospectral, and the diagonal entries of A^2 corresponding to cospectral vertices are equal. These are equal to their degrees. □

4.4 Walks Between Two Vertices

Let a and b be distinct vertices in X, and let $N_{b,a}(X,t)$ be the generating function for the walks in X from b to a that only use b once (necessarily at the start). We call these *non-returning walks*. Since any walk from b to a decomposes uniquely into a closed walk on b, followed by a non-returning walk from b to a:

4.4.1 Lemma. *If a and b are distinct vertices in X. then*

$$W_{b,a}(X,t) = W_{b,b}(X,t)N_{b,a}(X,t). \qquad \square$$

4.4.2 Lemma. *If a and b are distinct vertices in X, then*

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

Proof. The left side is the generating function for the walks in X that start at a and visit b at any point. Any such walk decomposes uniquely into a walk from a to b (with possible multiple visits at b), and a non-returning walk from b to a. Thus

$$W_{a,a}(X,t) - W_{a,a}(X \setminus b, t) = W_{a,b}(X,t)N_{b,a}(X,t)$$

and now the lemma follows using the previous lemma and the observation that $W_{a,b}(X,t) = W_{b,a}(X,t)$. □

Using Lemma 4.4.2 and Equation (4.3.3), and some straightforward manipulation, one arrives at the following corollary. We will be denoting the graph X with vertices a and b removed by $X \setminus ab$.

4.4.3 Theorem. *If a and b are distinct vertices in X, then*

$$t^{-1}W_{a,b}(X,t^{-1}) = \frac{(\phi(X \setminus a,t)\phi(X \setminus b,t) - \phi(X \setminus ab,t)\phi(X,t))^{1/2}}{\phi(X,t)}. \qquad \square$$

Further, as a consequence, we can recover a formula for the off-diagonal entries of E_r:

$$(E_r)_{a,b} = \left.\frac{(\phi(X \setminus a, t)\phi(X \setminus b, t) - \phi(X \setminus ab, t)\phi(X, t))^{1/2}(t - \theta_r)}{\phi(X, t)}\right|_{t=\theta_r}.$$

Let $\phi_{a,b}(X, t) = [\mathrm{adj}(tI - A)]_{a,b}$. Note that it is a polynomial. From Equation (4.3.2) and Theorem 4.4.3, it follows that

$$\phi_{a,b}(X, t) = (\phi(X \setminus a, t)\phi(X \setminus b, t) - \phi(X \setminus ab, t)\phi(X, t))^{1/2}.$$

We will refer to this as the *square-root identity*. Further, we can prove the following result.

4.4.4 Corollary. *Let $\mathcal{P}_{a,b}$ denote the collection of all paths between a and b. Then*

$$\phi_{a,b}(X, t) = \sum_{P \in \mathcal{P}_{a,b}} \phi(X \setminus P, t).$$

Proof. Note that $X \setminus P$ is the graph we get from X by deleting the **vertices** of P.

This will be a proof by induction on the number vertices of the graph. For graphs with 2 vertices, it follows trivially (provided you get the trivial cases right.) Now, consider non-returning walks from a to b, and their corresponding generating function $N_{a,b}(X, t)$. As we well know,

$$W_{a,a}(X, t^{-1})N_{a,b}(X, t^{-1}) = W_{a,b}(X, t^{-1}).$$

On the other hand,

$$N_{a,b}(X, t^{-1}) = t^{-1} \sum_{c \sim a} W_{c,b}(X \setminus a, t^{-1}).$$

By induction,

$$t^{-1}W_{c,b}(X \setminus a, t^{-1}) = \frac{1}{\phi(X \setminus a, t)} \sum_{P \in \mathcal{P}(X \setminus a)_{c,b}} \phi((X \setminus a) \setminus P, t).$$

Hence

$$\begin{aligned}\phi_{a,b}(X, t) &= t^{-1}W_{a,b}(X, t^{-1})\phi(X, t) \\ &= \frac{W_{a,a}(X, t^{-1})}{t\phi(X \setminus a, t)} \sum_{c \sim a} \sum_{P \in \mathcal{P}(X \setminus a)_{c,b}} \phi((X \setminus a) \setminus P, t)\phi(X, t).\end{aligned}$$

Result now follows from Equation (4.3.3). □

We also can derive the following consequence.

4.4.5 Corollary. *If there is a pair of cospectral vertices in X, then $\phi(X,t)$ is reducible over $\mathbb{Q}$.*

Proof. By Theorem 4.4.3

$$\phi_{a,b}(X,t)^2 = \phi(X\setminus a,t)\phi(X\setminus b,t) - \phi(X\setminus ab,t)\phi(X,t).$$

If a and b are cospectral this implies that

$$\begin{aligned}\phi(X\setminus ab,t)\phi(X,t) &= \phi(X\setminus a,t)^2 - \phi_{a,b}(X,t)^2\\ &= (\phi(X\setminus a,t) - \phi_{a,b}(X,t))(\phi(X\setminus a,t) + \phi_{a,b}(X,t)).\end{aligned}$$

As each factor in this expression has degree at most $|V(X)|-1$, we conclude that $\phi(X,t)$ has a non-trivial factor over $\mathbb{Q}$. □

4.5 The Jacobi Trick

If $D\subseteq V(X)$ and M is a square matrix with rows and columns indexed by $V(X)$, then $M_{D,D}$ shall denote the square submatrix of M with rows and columns indexed by D. The following theorem is due to Jacobi.

4.5.1 Theorem. *Let X be a graph. If $D\subseteq V(X)$, then*

$$\det\,((tI-A)^{-1})_{D,D} = \frac{\phi(X\setminus D,t)}{\phi(X,t)}.$$

Proof. Assume for convenience that vertices corresponding to D are the first rows and columns of A. Let M be the matrix formed by replacing the first d columns of the $n\times n$ identity matrix with the corresponding columns of $(tI-A)^{-1}$. We can write M in partitioned form

$$M = \begin{pmatrix} M_1 & 0\\ M_2 & I\end{pmatrix}$$

where $M_1 = ((tI-A)^{-1})_{D,D}$ and the details of M_2 are irrelevant. Then

$$(tI-A)M = \begin{pmatrix} I & N_1\\ 0 & tI-A(X\setminus D)\end{pmatrix}$$

and hence

$$\det(tI - A)\det(M_1) = \det(tI - A(X \setminus D)). \qquad \square$$

This can be used to give an alternate proof of Theorem 4.4.3, which you are invited to find as an exercise.

4.5.2 Corollary. *Let $\theta_0, \dots, \theta_d$ be the distinct eigenvalues of X, with corresponding spectral idempotents $E_0, \dots, E_d$. If $D \subseteq V(X)$, the multiplicity of θ_r as a pole of $\phi(X \setminus D, t)/\phi(X, t)$ is equal to $\operatorname{rk}((E_r)_{D,D})$.*

Proof. We have

$$((tI - A)^{-1})_{S,S} = \sum_{r=0}^{d} \frac{1}{t - \theta_r}(E_r)_{S,S}.$$

Let $F_i = (t - \theta_i)^{-1}(E_i)_{S,S}$, and let P be an orthogonal matrix such that $D = P^T(E_i)_{S,S}P$ is diagonal. Let $H = \sum_{i:i \neq r} F_i$. Thus,

$$\frac{\phi(X \setminus S, t)}{\phi(X, t)} = \det\left(\frac{1}{t - \theta_r}D + P^T H P\right).$$

From the Laplace expansion, this determinant is the sum of the determinants of the matrices we obtain from $P^T H P$ by replacing each subset of columns by the corresponding set from $(t - \theta_r)^{-1}D$. The non-zero diagonal entries of this matrix contain poles at θ_s, but the entries of $P^T H P$ do not. Thus, selecting precisely the set of columns corresponding to the non-zero columns of D will provide a unique term in the determinant expansion whose multiplicity of the pole at θ_s is precisely the rank of $(E_s)_{D,D}$. $\square$

The following argument is due to Xiaohong Zhang.

4.5.3 Lemma. *Vertices a and b of X are parallel if and only if the poles of $\phi(X \setminus \{a, b\}, t)/\phi(X, t)$ are simple.*

Proof. Let θ_r be an eigenvalue of X. We have

$$(E_r)_{a,a} = \left.\frac{\phi(X \setminus a, t)(t - \theta_r)}{\phi(X, t)}\right|_{t=\theta_r}, \qquad (E_r)_{b,b} = \left.\frac{\phi(X \setminus b, t)(t - \theta_r)}{\phi(X, t)}\right|_{t=\theta_r}$$

and

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

Now

$$\det\begin{pmatrix}(E_r)_{a,a} & (E_r)_{a,b}\\ (E_r)_{a,b} & (E_r)_{b,b}\end{pmatrix} = (E_r)_{a,a}(E_r)_{b,b} - (E_r)_{a,b}^2$$
$$= \left.\frac{\phi(X\setminus\{a,b\},t)(t-\theta_r)^2}{\phi(X,t)}\right|_{t=\theta_r}$$

and, if the multiplicity of θ_r in $\phi(X,t)$ is m, last term is not zero if and only the multiplicity of θ_r in $\phi(X\setminus\{a,b\},t)$ is $m-2$. (By interlacing, it cannot be less.) Since a and b are parallel if and only if the determinant is zero, the result follows. □

4.6 All Walks

The generating function whose coefficients of t^k count all walks of length k in X is

$$\operatorname{sum}(W(X,t)) = \sum_{r=0}^{d}\frac{\mathbf{1}^T E_r \mathbf{1}}{1-t\theta_r}.$$

Note that, for regular graphs, this says that the generating function of all walks depend only on the valency and the size of the graph. We will see in this section how that this can be expressed in general using $\phi(X,t)$ and $\phi(\overline{X},t)$. The following lemma is a well known fact.

4.6.1 Lemma. *For any matrices M and N such that MN and NM are defined,*

$$\det(I-MN) = \det(I-NM).$$

Proof. Follows immediately from

$$\begin{pmatrix}I & M\\ 0 & I\end{pmatrix}\begin{pmatrix}I-MN & 0\\ N & I\end{pmatrix} = \begin{pmatrix}I & M\\ N & I\end{pmatrix} = \begin{pmatrix}I & 0\\ N & I\end{pmatrix}\begin{pmatrix}I & M\\ 0 & I-NM\end{pmatrix}.$$

□

4.6.2 Theorem. *For any graph X on n vertices,*

$$\frac{\phi(\overline{X},t)}{(-1)^n\phi(X,-t-1)} = 1 - \sum_{r=0}^{d}\frac{\mathbf{1}^T E_r \mathbf{1}}{t+1+\theta_r} = 1 - \mathbf{1}^T((t+1)I+A)^{-1}\mathbf{1}.$$

Proof. We have

$$tI - A(\overline{X}) = (t+1)I + A - J = ((t+1)I + A)(I - ((t+1)I + A)^{-1}J).$$

Applying the lemma,

$$\begin{aligned}\det(I - ((t+1)I + A)^{-1}J) &= \det(I - ((t+1)I + A)^{-1}\mathbf{1}\mathbf{1}^T) \\ &= 1 - \mathbf{1}^T((t+1)I + A)^{-1}\mathbf{1}.\end{aligned}$$

The result now follows using this and the spectral decomposition of $((t+1)I + A)^{-1}$. □

Cospectral pairs of regular graphs have their complements cospectral. The following corollary is, in a sense, the right generalization of this fact applied to non-regular graphs.

4.6.3 Corollary. *Suppose X and Y are cospectral. Then $\overline{X}$ and $\overline{Y}$ are cospectral if and only if*

$$\operatorname{sum}(W(X,t)) = \operatorname{sum}(W(Y,t)).$$ □

A similar approach can be taken to study all walks at a vertex. If $a \in V(X)$, let $W_a(X,t)$ be the generating function for the walks in X that start at a, and let $N_a(X,t)$ be the generating function for the non-returning walks that start at a. Then

$$t^{-1}W_a(X,t^{-1}) = \sum_{r=0}^{d} \frac{e_a^T E_r \mathbf{1}}{t - \theta_r}$$

and, also,

$$W_a(X,t) = W_{a,a}(X,t)N_a(X,t).$$

4.6.4 Lemma. *If $a \in V(X)$, then*

$$\operatorname{sum}(W(X,t)) - \operatorname{sum}(W(X \setminus a,t)) = \frac{W_a(X,t)^2}{W_{a,a}(X,t)}$$

Proof. The left side of our proposed identity is the generating function for the walks in X that use a at any point. Such walks can be split into those a walk in X that starts somewhere and arrives at a, followed by a closed walk on a, and which ends with a non-returning walk starting at a. Hence the generating function for these walks factors as

$$N_a(X,t)W_{a,a}(X,t)N_a(X,t),$$

and our lemma follows. □

We say that two pairs (X, a) and (Y, b) are *cospectral with cospectral complements* if X and Y are cospectral with cospectral complements and $X \setminus a$ and $Y \setminus b$ are cospectral with cospectral complements.

Applying the results of the past section X and $X \setminus a$, and the lemma above, we get

$$t^{-1}W_a(X, t^{-1}) = \left((-1)^n \frac{\phi(X \setminus a, t)}{\phi(X, t)} \left(\frac{\phi(\overline{X}, -t-1)}{\phi(X, t)} + \frac{\phi(\overline{X} \setminus a, -t-1)}{\phi(X \setminus a, t)}\right)\right)^{1/2}. \tag{4.6.1}$$

As a consequence, the corollary below follows.

4.6.5 Corollary. *Suppose $a, b \in V(X)$ and $X \setminus a$ and $X \setminus b$ are cospectral. Then the $\overline{X} \setminus a$ and $\overline{X} \setminus b$ are cospectral if and only if*

$$W_a(X, t) = W_b(X, t). \qquad \square$$

4.7 1-Sums and 2-Sums

Suppose X and Y are graphs, and let Z be the graph we get by identifying a vertex of X with a vertex of Y. Equivalently, we may assume that $V(X) \cap V(Y) = \{a\}$ and no edge joins a vertex of $X \setminus a$ with a vertex of $Y \setminus a$. We say Z is a *1-sum* of X and Y at a.

For any graph X with vertex a, let $C_a(X, t)$ be the generating function for the closed walks on a that return exactly once. All walks that start and end at a can be decomposed into a walk that starts and ends at a, followed by another that start at a and returns exactly once. Thus

$$W_{a,a}(X, t)(1 - C_a(X, t)) = 1,$$

and therefore

$$C_a(X, t) = 1 - W_{a,a}(X, t)^{-1}.$$

4.7.1 Lemma. *If Z is the 1-sum of X and Y at a, then*

$$\phi(Z, t) = \phi(X \setminus a, t)\phi(Y, t) + \phi(X, t)\phi(Y \setminus a, t) - t\phi(X \setminus a, t)\phi(Y \setminus a, t)$$

Proof. We have

$$C_a(Z, t) = C_a(X, t) + C_a(Y, t).$$

The rest follows from Equation (4.3.3). $\square$

It follows that the spectrum of the 1-sum of X and Y at a is determined by the spectra of the four graphs X, $X \setminus a$, Y, and $Y \setminus a$. Since

$$W_a(Z,t) = W_{a,a}(Z,t)N_a(Z,t) = W_{a,a}(Z,t)(N_a(X,t) + N_a(Y,t) - 1),$$

it follows that the spectrum of $\overline{Z}$ is determined by the spectra of the four graphs above, and the spectra of their complements.

If a and b are cospectral vertices in X and $c \in V(Y)$, then the 1-sum of (X,a) and (Y,c) is cospectral to the 1-sum of (X,b) and (Y,c). Schwenk used this construction as part of his proof that the proportion of trees on n vertices that are determined by their characteristic polynomials tends to zero as n increases.

We note one consequence of the previous lemma.

4.7.2 Corollary. *Let X and Y be vertex-disjoint graphs and let a be a vertex in X and b a vertex in Y. If Z is the graph we get from $X \cup Y$ by adding an edge joining a to b, then*

$$\phi(Z,t) = \phi(X,t)\phi(Y,t) - \phi(X \setminus a, t)\phi(Y \setminus b, t). \qquad \square$$

One way to prove this is apply Lemma 4.7.1 twice, first forming the 1-sum of X and K_2, then taking the 1-sum of this with Y.

We form the *2-sum* of graphs X and Y by merging a pair of vertices in X with a pair of vertices in Y. In any interesting case the merged pair of vertices form a cutset in the 2-sum. To carry out our discussion, we assume we have a graph Z with non-adjacent vertices a and b and subgraphs X and Y such that

$$V(X) \cup V(Y) = V(Z), \quad V(X) \cap V(Y) = \{a,b\}.$$

Thus Z is a 2-sum of X and Y and we want to relate the spectrum of Z to that of X and Y. We note that a path in Z from a to b must lie in X or in Y. Hence, by Corollary 4.4.4,

$$\phi_{a,b}(Z,t) = \phi_{a,b}(X,t)\phi(Y \setminus ab, t) + \phi_{a,b}(Y,t)\phi(X \setminus ab, t),$$

and consequently

$$\begin{aligned}\phi(Z \setminus ab, t)\phi(Z,t) = {} & \phi(Z \setminus a, t)\phi(Z \setminus b, t) \\ & - (\phi_{a,b}(X,t)\phi(Y \setminus ab, t) + \phi_{a,b}(Y,t)\phi(X \setminus ab, t))^2.\end{aligned}$$

Since $Z \setminus a$ and $Z \setminus b$ are 1-sums, we can express their characteristic polynomials in terms of characteristic polynomials of the subgraphs

$$X \setminus a,\ X \setminus b,\ X \setminus ab,\ Y \setminus a,\ Y \setminus b,\ Y \setminus ab.$$

So we have a formula of sorts for $\phi(Z, t)$.

Our work in this section provides the following result.

4.7.3 Theorem. *The 2-sum of graphs X and Y at a pair of cospectral vertices, a and b, which are not neighbours, yields a graph Z where a and b are not neighbours and are cospectral.*

Proof. Note that $Z \setminus a$ is the 1-sum of $X \setminus a$ and $Y \setminus a$ at the vertex b, so

$$\phi(Z\setminus a, t) = \phi(X\setminus a, t)\phi(Y\setminus ab, t) + \phi(X\setminus ab, t)\phi(Y\setminus a, t) - t\phi(X\setminus ab, t)\phi(Y\setminus ab, t)$$

and, likewise

$$\phi(Z\setminus b, t) = \phi(X\setminus b, t)\phi(Y\setminus ab, t) + \phi(X\setminus ab, t)\phi(Y\setminus b, t) - t\phi(X\setminus ab, t)\phi(Y\setminus ab, t).$$

Therefore

$$\begin{aligned}\phi(Z \setminus a, t) - \phi(Z \setminus b, t) = \phi(X \setminus a, t)\phi(Y \setminus ab, t) + \phi(X \setminus ab, t)\phi(Y \setminus a, t) \\ - \phi(X \setminus b, t)\phi(Y \setminus ab, t) - \phi(X \setminus ab, t)\phi(Y \setminus b, t)\end{aligned}$$

and, thus, a and b are cospectral in Z if and only if

$$\frac{\phi(X \setminus a, t)}{\phi(X \setminus ab, t)} - \frac{\phi(X \setminus b, t)}{\phi(X \setminus ab, t)} = \frac{\phi(Y \setminus b, t)}{\phi(Y \setminus ab, t)} - \frac{\phi(Y \setminus a, t)}{\phi(Y \setminus ab, t)}.$$

It follows that if a and b are cospectral in X and in Y, then they are cospectral in their 2-sum Z. □

4.8 Reduced Walks

A walk in a graph X is *reduced* if it does not contain a subsequence of the form aba. (Sometimes these are called *non-backtracking* walks.) If $|V(X)| = n$, then the matrix generating series $\Phi(X, t)$ is defined by declaring that $\Phi(X, t))_{a,b}$ is the generating series for the reduced walks in X from a to b, for all vertices a and b of X. We see that if X is a tree, there is exactly one reduced walk between a given pair of vertices, and the length of the walk is the distance between the vertices. Hence if T is a tree, the entries of $\Phi(T,t)$ are polynomials of degree at most the diameter of T. Equivalently we can write

$$\Phi(T,t) = \sum_{r\geq 0} t^r A_r,$$

where $(A_r)_{a,b} = 1$ if $\operatorname{dist}(a,b) = r$ and is otherwise zero. If T is a tree, then $\Phi'(T,1) = D(T)$, where $D(T)$ is the distance-matrix of T.

If $A = A(X)$, define $p_r(A)$ to be the matrix (of the same order as A) such that $(p_r(A))_{a,b}$ is the number of reduced walks in X from a to b of length r. Thus

$$\Phi(X,t) = \sum_{r\geq 0} t^r p_r(A).$$

Observe that

$$p_0(A) = I, \quad p_1(A) = A, \quad p_2(A) = A^2 - \Delta,$$

where Δ is the diagonal matrix of valencies of X. If $r \geq 3$ we have the recurrence

$$Ap_r(A) = p_{r+1}(A) + (\Delta - I)p_{r-1}(A).$$

These calculations were first carried out by Biggs, who observed the implication that $p_r(A)$ is a polynomial in A and Δ, of degree r in A. Our next theorem combines two results from Chan and Godsil [18].

4.8.1 Theorem. *For any graph X on at least two vertices,*

$$\Phi(X,t)(I - tA + t^2(\Delta - I)) = (1-t^2)I.$$

Furthermore, $\det(I - tA + t^2(\Delta - I)) = 1 - t^2$ *if and only if X is a tree.* □

4.9 Hermitian Matrices

In defining $U(t)$, the key constraint on A is that it be Hermitian. Most of the theory presented in this chapter extends without great difficulty to this case, and we describe briefly how to do this here.

We start with a square matrix M with entries from some commutative ring and with its rows and columns indexed by some set V. We define a walk relative to M to be a sequence of ordered pairs of vertices of X, such that the tail of one term is the head of the term immediately following. The weight of the vertex pair (a, b) is $M_{a,b}$, and the weight of a walk is the product of the weights of its terms. The generating function for walks on M is

$$(I - tM)^{-1} = \sum_{k \geq 0} t^k M^k$$

and the coefficient of t^k in $((I - tM)^{-1})_{a,b}$ is the sum of the weights of the walks of length k starting at a and ending at b. When $V = V(X)$ for some graph X, we might view M as a weighted adjacency matrix for X; in this case we assume that $M_{a,b} = 0$ if $ab \notin E(X)$.

If $M[a, b]$ denotes the matrix we get by deleting the a-row and b-column from M, then, from adjugate expression for the inverse,

$$((I - tM)^{-1})_{a,b} = \frac{\det((I - tM)[a, b])}{\det(I - tM)}.$$

The identities derived in this chapter extend routinely to the case where M is Hermitian. (They can also extend to the case where M is a normal matrix.) For example, in Corollary 4.4.4, we related an off diagonal entry of $(I - t^{-1}A)^{-1}$ with paths. If instead of A we have an Hermitian matrix M, then we proceed as follows. If α is a walk in X, let $\mathrm{wt}(\alpha)$ denote its weight. If P is a path in X from a to b, we can view it as a walk and hence it has a weight $\mathrm{wt}(P)$. If M is Hermitian, the weight of a walk from b to a is the complex conjugate of the weight of the reversed walk from b to a.

4.9.1 Theorem. *Let M be a Hermitian weighted adjacency matrix for X and let a and b be distinct vertices in X. Let $\mathcal{P}$ denote the set of paths in X from a to b. Then*

$$t^{-1}((I - t^{-1}M)^{-1})_{a,b} = \sum_{P \in \mathcal{P}} \mathrm{wt}(P) \frac{\phi(M \setminus P, t)}{\phi(M, t)}. \qquad \square$$

4.10 No Transfer at all on Some Signed Graphs

We use the ideas from the previous section to study state transfer on signed graphs. A signed adjacency matrix for a graph is symmetric and its nonzero entries are 1 or −1. Let C be the cycle C_4 with signed adjacency matrix

$$A = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}.$$

We claim that if $U(t) = \exp(itA)$, then $U(t)_{1,2} = 0$ for all t. To prove this, we first observe that the vertices 1 and 2 are joined by exactly two paths, each of length two and with one of weight 1 and the other with weight −1.

If P is either of these paths, then $\phi(C \setminus P) = t$ and therefore, by Theorem 4.9.1, we have that $((tI - A)^{-1})_{1,2} = 0$.

Accordingly

$$0 = \sum_{r=0}^{d} \frac{(E_r)_{1,2}}{t - \theta_r}$$

and therefore $(E_r)_{1,2} = 0$ for all r. Since

$$U(t)_{1,2} = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} (E_r)_{1,2}$$

we conclude that $U(t)_{1,2} = 0$ for all t.

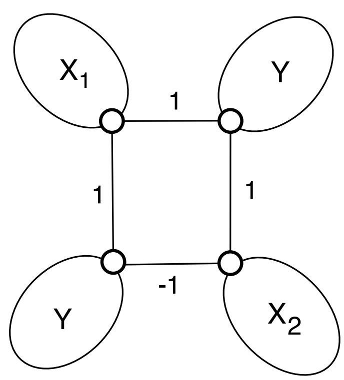

Figure 4.1: A graph with no transfer from X_1 to X_2

Now construct a graph Z as follows. Choose rooted graphs X_1, X_2 and Y and let Z be the graph by merging the roots of X_1, X_2 and two copies of Y with the vertices of C_4, to produce the signed graph shown in Figure 4.10.

Let W be the graph that we get when X_1 and X_2 are both K_1. Let 1 and 2 denote the images of the root vertices of X_1 and X_2 in Z and let a be a vertex in X_1 and b a vertex in X_2. Sign the edges as in the figure. Then by the result in Exercise 1, we have

$$\phi_{a,b}(Z,t) = \phi_{a,1}(X_1,t)\phi_{1,2}(W,t)\phi_{2,b}(X_2,t)$$

and since any 12-path in W uses only vertices in C, our signing ensures that $\phi_{1,2}(W,t) = 0$. Therefore $\phi_{a,b}(Z,t) = 0$ and thus it follows that $U_Z(t)_{a,b} = 0$ for all t.

The example above provides a refined explanation of why in certain signed graphs there can be no transfer. However, the example above can be cast in a general setting as follows. The key property of C, the signed C_4, is that it is bipartite and that its adjacency matrix has the form

$$A = \begin{pmatrix} 0 & H \\ H^T & 0 \end{pmatrix}$$

and $HH^T = 2I$. So assume X is a graph with signed adjacency matrix of this form, where H is a square and $HH^T = kI$. (For example H could be a Hadamard or a conference matrix.) Then $(k^{-1/2}A)^2 = I$ and so

$$\exp(\mathrm{i}tk^{-1/2}A) = \cos(t)I + \mathrm{i}k^{-1/2}\sin(t)A.$$

If follows that a and b are two vertices in the same color class of X, then $U(t)_{a,b} = 0$ for all t. By taking 1-sums we can construct more examples with no transfer.

Notes

The results in this Chapter are in large part an extension of results from [35, Chapter 4].

Karimipour, Rad and Asoudeh study a construction related to the one in Section 4.10 in [44],

Exercises

4-1. Suppose Z is the 1-sum of graphs X and Y using a vertex a. If b and c are vertices in $X \setminus a$ and $Y \setminus b$ respectively, show that

$$\phi_{b,c}(Z,t) = \phi_{b,a}(X,t)\phi_{a,c}(Y,t).$$

4-2. Prove Theorem 4.4.3 in two different ways.

Chapter 5

Walk Modules

Suppose e_S is the characteristic vector of a subset S of the vertices of the graph X. Then, to put things in their simplest terms, in this chapter we investigate the A-invariant subspace spanned by the vectors $A^r e_S$, for all non-negative r. In more high flown terms, this subspace is the cyclic $\mathbb{R}[A]$-module generated by e_S. Properties of these modules will be particularly useful in our study of quantum walks in graphs.

In a quantum information context, x represents a initial state, typically $x = e_a$ when S contains a single vertex a. Then the Hamiltonian, given by $A = A(X)$, yields an evolution given by $U(t)$, which is a polynomial in A. Therefore, for any t, the resulting quantum state lies in the $\mathbb{R}[A]$-module generated by x.

5.1 Walk Modules

Let X be a graph on n vertices and let S be a subset of $V(X)$ with characteristic vector e_S. The *walk matrix* relative to S is

$$W_S := \begin{pmatrix} e_S & Ae_S & \dots & A^{n-1}e_S \end{pmatrix}.$$

The column space of W_S is the A-invariant subspace of $\mathbb{R}^n$ generated by e_S. Equivalently, if $\mathbb{R}[A]$ denotes the ring (or algebra) of all polynomials in A, then $\operatorname{col}(W_S)$ is the $\mathbb{R}[A]$-module generated by e_S, and therefore we call it the *walk module* of S. We might also abuse both notations at once and refer to it as the A-module generated by e_S.

Note that

$$(W_S^T W_S)_{i,j} = (e_S)^T A^{i-1} A^{j-1} e_S = (e_S)^T A^{i+j-2} e_S$$

and therefore $(W_S^T W_S)_{i,j}$ is the number of walks in X of length $i+j-2$ that start and finish on a vertex in S. Let $C_S(X,t)$ be the generating series for the walks in X that start and finish at a vertex in S. Then $C_S(X,t)$ determines the product $W_S^T W_S$, and it is not too hard to show that entries of $W_S^T W_S$ suffice to determine $C_S(X,t)$. Moreover:

5.1.1 Lemma. *If S is a nonempty subset of $V(X)$, then*

$$C_S(X,t) = \sum_{r=0}^{d} \frac{e_S^T E_r e_S}{1 - t\theta_r},$$

□

If $z \in \mathbb{R}^n$, then the *minimal polynomial* of A relative to z is the monic polynomial p of least degree such that $p(A)z = 0$. If ψ is the usual minimal polynomial of A, then $\psi(A)z = 0$ (without doubt) and so, as a consequence of Euclidean division, we have that p divides ψ. It is an exercise to show that the degree of the minimal polynomial of A relative to x_S equals $\mathrm{rk}(W_S)$.

5.2 Dual Degree and Covering Radius

Let $E_0, \ldots, E_d$ be the idempotents in the spectral decomposition of A. Then

$$A^k = \sum_{r=0}^{d} \theta_r^k E_r$$

and therefore the vectors $A^k e_S$ are generated by the $\{E_r e_S\}_{r=0}^d$. On the other hand, since each E_r is a polynomial in A, it follows that each $E_r x_s$ is a combination of the columns of W_S. We conclude that

$$\mathrm{col}(W_S) = \langle \{E_r e_s\}_{r=0}^d \rangle,$$

and thus, as the $\{E_r e_s\}_{r=0}^d$ are orthogonal, we have

$$\mathrm{rk}(W_S) = |\{\theta_r : E_r e_S \neq 0\}|.$$

We define the *dual degree* of S to be $\mathrm{rk}(W_S) - 1$. If X is connected and E_0 is the idempotent belonging to the spectral radius, then all entries of E_0 are positive. Hence the dual degree of a non-empty subset of $V(X)$ is non-negative. The terminology "dual degree" comes from coding theory: if X is the Hamming graph $H(n,q)$ with vertex set $GF(q)^n$ and S is a linear code then the dual degree of S is the degree of its dual code.

The set of eigenvalues θ_r such that $E_r e_S \neq 0$ is the *eigenvalue support* of S. Since

$$e_S^T E_r e_S = e_S^T E_r^2 e_S = e_S^T E_r^T E_r e_S = \|E_r e_S\|^2,$$

we find that $E_r e_S = 0$ if and only if $e_S^T E_r e_S = 0$. If X is connected then the support of any non-empty subset of $V(X)$ contains the spectral radius.

5.2.1 Lemma. *The eigenvalue support of a vertex set a of X consists of the eigenvalues θ_r such that θ_r is a pole of the rational function $\phi(X \setminus a, t)/\phi(X,t)$.*

Proof. From Equation (4.3.4),

$$\phi(X \setminus a, t)/\phi(X,t) = \sum_{r=0}^{d} \frac{(E_r)_{a,a}}{t - \theta_r},$$

whence the result follows. □

5.2.2 Corollary. *If θ belongs to the eigenvalue support of a, then so do all algebraic conjugates of θ.* □

5.2.3 Lemma. *If a and b are distinct vertices in X and $(E_r)_{a,b} \neq 0$, then θ_r lies in the eigenvalue supports of both a and b.*

Proof. We have

$$(E_r)_{a,b} = \langle E_r e_a, E_r e_b \rangle$$

and therefore by Cauchy-Schwarz,

$$|(E_r)_{a,b}| \leq \|E_r e_a\| \, \|E_r e_b\|.$$ □

5.2.4 Lemma. *If X is bipartite, the eigenvalue support of a vertex is closed under multiplication by -1,* *Proof.* We may assume X is connected. Let D be a diagonal matrix with diagonal entries equal to 1 on one colour class and equal to -1 on the other. Then $DAD = -A$ and if $Az = \theta z$, then $-\theta z = DADz$ and so Dz is an eigenvector with eigenvalue $-\theta$. The lemma follows. □

The *covering radius* of S is the least integer r such that any vertex of X is a distance at most r from S. Thus S is a dominating set if and only if its covering radius is 1, and the diameter of a graph is the maximum value of the covering radii of the vertices. (The covering radius of a vertex is also known as the *eccentricity* of the vertex.) Our next lemma generalizes the well known fact that if X has diameter d, then the number of distinct eigenvalues of X is at least $d + 1$.

5.2.5 Lemma. *If S is a non-empty subset of $V(X)$ with covering radius r and dual degree s^*, then $r \leq s^*$.*

Proof. If e_S is the characteristic vector of S, then for $k = 0, \ldots, r$ the supports of the vector $(A+I)^k e_S$ are strictly increasing and therefore these vectors are linearly independent. □

As an example, if X is the path P_n on n vertices and S is one of its end-vertices, then covering radius of S is $n-1$. Hence the dual degree of an end vertex is $n-1$, from which we deduce the well known fact that the eigenvalues of the path are distinct.

5.3 Controllable Pairs, Symmetries, Rational Functions

Let X be a graph on n vertices with adjacency matrix A. If $z \in \mathbb{R}^n$, define the matrix W_z by

$$W_z = \begin{pmatrix} z & Az & \ldots & A^{n-1}z \end{pmatrix}.$$

The pair (A, z) is said to be *controllable* if W_z is invertible. In this chapter, z will often be the characteristic vector e_S of some subset S of $V(X)$, and then we will say that (X, S) is controllable if (A, e_S) is. Note that, given A, if there is z so that (A, z) is controllable, then A must have simple eigenvalues. This observation implies the following result, recalling that the only vertex transitive graph with all eigenvalues simple is K_2.

5.3.1 Corollary. *If X is vertex transitive and $|V(X)| > 2$, no subset of $V(X)$ is controllable.*

We can also relate another aspect of symmetries to controllability.

5.3.2 Lemma. *If (X, S) is controllable, then any automorphism of X that fixes S as a set is the identity.*

Proof. Let P be a permutation matrix that commutes with A (thus P defines an automorphism of X). It fixes S if and only if $Pe_S = e_S$. Hence, in this case,

$$PA^r e_S = A^r P e_S = A^r e_S,$$

and therefore $PW_S = W_S$. Hence if W_S is invertible, $P = I$. □

We derive some useful characterizations of controllability. From the spectral decomposition of A, we see that

$$(tI - A)^{-1} z = \sum_{r=0}^{d} \frac{1}{t - \theta_r} E_r z$$

and hence

$$z^T (tI - A)^{-1} z = \sum_{r=0}^{d} \frac{z^T E_r z}{t - \theta_r}. \tag{5.3.1}$$

Since

$$z^T E_r z = z^T E_r^2 z = (E_r z)^T E_r z, \tag{5.3.2}$$

we have that $z^T E_r z = 0$ if and only if $E_r z = 0$. Therefore the rank of W_z is equal to the number of distinct poles of the rational function $z^T (tI - A)^{-1} z$. With $z = e_S$ for some subset $S \subseteq V(X)$, then there is a polynomial $\phi_S(X, t)$ with degree at most $n - 1$ such that

$$e_S^T (tI - A)^{-1} e_S = \frac{\phi_S(X, t)}{\phi(X, t)}$$

(As we have already seen, if S is the vertex a, then $\phi_S(X, t) = \phi(X \setminus a, t)$.)

This provides a useful characterization of controllability:

5.3.3 Lemma. *Let X be a graph on n vertices and suppose $S \subseteq V(X)$, with characteristic vector e_S. Then (X, S) is controllable if and only if the rational function $e_S^T (tI - A)^{-1} e_S$ has n distinct poles.* □

We have the following consequence of Lemma!5.3.3 and the remark preceding it:

5.3.4 Corollary. *A vertex a in X is controllable if and only if $\phi(X \setminus a, t)$ and $\phi(X, t)$ are coprime.* □

For the path P_n on n vertices we have

$$\phi(P_0, t) = 1, \qquad \phi(P_1, t) = t$$

and, if $n \geq 1$,

$$\phi(P_{n+1}, t) = t\phi(P_n, t) - \phi(P_{n-1}, t)$$

from which it follows by induction that $\phi(P_{n+1}, t)$ and $\phi(P_n, t)$ are coprime for all n. So if a is an end-vertex of P_n, the pair $(P_n, \{a\})$ is controllable.

5.4 Controllable Subsets

Our next theorem will characterize controllability in terms of linear algebra rather than rational functions. First a useful lemma.

5.4.1 Lemma. *Let $v_1, \ldots, v_m$ be a set of vectors in $\mathbb{R}^n$, and let $Q_{ij} = v_i v_j^T$. Then $\{v_1, ..., v_m\}$ spans a subspace of dimension k if and only if $\{Q_{ij}\}_{i,j=1}^m$ spans a subspace of dimension k^2 in the space of $n \times n$ matrices with real entries.*

Proof. We show that $v_1, \ldots, v_k$ is linearly independent if and only if the k^2 matrices $v_i v_j^T$ for $\leq i, j \leq k$ are linearly independent.

If $v_1, \ldots, v_k$ are linearly dependent, the matrices $v_i v_1^T$ (for $i = 1, \ldots, k$) are linearly dependent.

So assume that $v_1, \ldots, v_k$ are linearly independent. Then there are vectors $u_1, \ldots, u_k$ such that $v_i^T u_j = \delta_{i,j}$. (The vectors $u_1, \ldots, u_k$ form a *dual basis*). Assume by way of contradiction that there are scalars $a_{i,j}$ such that

$$\sum_{1 \leq i,j \leq k} a_{i,j} v_i v_j^T = 0.$$

Then

$$0 = u_r^T \left(\sum_{1 \leq i,j \leq k} a_{i,j} v_i v_j \right) u_s = \sum_{1 \leq i,j \leq k} a_{i,j} (u_r^T v_i)(v_j^T u_s) = a_{r,s}.$$

Therefore the matrices $v_i v_1^T$ are linearly independent. □

As an immediate consequence, we get:

5.4.2 Corollary. *Let S be a subset of the vertices of the graph X, with characteristic vector $z = e_S$. The following statements are equivalent:*

(a) *(X, S) is controllable.*

(b) *The matrices $A^i zz^T A^j$ where $0 \leq i, j < n$ form a basis for the algebra of all $n \times n$ matrices.* □

We can also express things in terms of the algebra $\langle A, zz^T \rangle$ generated by A and zz^T.

5.4.3 Theorem. *Assume A is an $n \times n$ real matrix and $z \in \mathbb{R}^n$. Then A and zz^T generate $\mathrm{Mat}_{n\times n}(\mathbb{R})$ if and only if the matrices $A^i zz^T A^j$, where $0 \leq i, j < n$, are linearly independent.*

Proof. Since $\dim(\mathrm{Mat}_{n\times n}(\mathbb{R})) = n^2$, if the matrices given are linearly independent they form a basis for $\mathrm{Mat}_{n\times n}(\mathbb{R})$.

So we assume that $\langle A, zz^T \rangle = \mathrm{Mat}_{n\times n}(\mathbb{R})$. By Lemma 5.4.1, it is enough to show that the vectors $z, Az, \ldots, A^{n-1}z$ are linearly independent. Let W denote the span of these vectors. By the Cayley-Hamilton theorem, A^n is a linear combination of the powers A^k for $k0, \ldots, n-1$ and therefore W is invariant under A. Since

$$zz^T A^k z = (z^T A^k z)z \in W,$$

it is also invariant under zz^T. Consequently W is invariant under $\mathrm{Mat}_{n\times n}(\mathbb{R})$ and therefore $\dim(W) = n$. □

If $S \subseteq V(X)$, we define the *cone of X relative to S* to be the graph we get by taking a new vertex, say 0, and joining it to each vertex in S, and denote it by $\widehat{X_S}$.

5.4.4 Lemma. *Let $S \subseteq V(X)$. Then*

$$\phi(\widehat{X_S}, t) = \phi(X, t)(t - e_S^T (tI - A)^{-1} e_S).$$

Proof. This follows from

$$\begin{pmatrix} t & -e_S^T \\ -e_S & (tI - A) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & (tI - A) \end{pmatrix} \begin{pmatrix} t & -e_S^T \\ -(tI - A)^{-1} e_S & I \end{pmatrix}.$$ □

5.4.5 Theorem. *Let X be a graph and $S \subseteq V(X)$. Then (X,S) is controllable if and only if $(\widehat{X_S}, \{0\})$ is controllable.*

Proof. The lemma implies that

$$\frac{\phi(\widehat{X_S}, t)}{\phi(X,t)} = t - \sum_{r=0}^{d} \frac{e_S^T E_r e_S}{t-\theta_r}. \tag{5.4.1}$$

Further, Lemma 5.3.3 says that (X,S) is controllable if and only if this rational function has n distinct poles. Now

$$e_0^T(tI-\widehat{A})^{-1}e_0 = \Big((tI-\widehat{A})^{-1}\Big)_{0,0} = \frac{\phi(X,t)}{\phi(\widehat{X},t)}$$

and therefore $(\widehat{X_S}, \{0\})$ is controllable if and only if the rational function $\phi(X,t)/\phi(\widehat{X_S},t)$ has $n+1$ distinct poles, that is, if and only if $\phi(\widehat{X_S},t)/\phi(X,t)$ has exactly $n+1$ distinct zeros.

Since the derivative of the right side in (5.4.1) is positive everywhere it is defined, between each pair of consecutive zeros there is exactly one pole. Therefore there are $n+1$ distinct zeros. □

The following corollary provides infinite families of controllable pairs.

5.4.6 Corollary. *Let S be a subset of $V(X)$, and let Y_k be the graph obtained by taking a path on k vertices and joining one of its end-vertices to each vertex in S. Let 0 denote the other end-vertex of the path. If (X,S) is controllable then $(Y_k,\{0\})$ is controllable.* □

5.5 Controllable Graphs

We say that graph is *controllable* if $(X, V(X))$ is controllable.

Theorem 5.4.3 readily implies the following corollary.

5.5.1 Corollary. *A graph is controllable if and only if its complement is.* □

Since any automorphism of X fixes $V(X)$, we see that a controllable graph is asymmetric, as per Lemma 5.3.2.

Moreover, assume X and Y are isomorphic, with adjacency matrices A and B respectively. For some permutation matrix P we have $B = P^T AP$. As an immediate consequence,

$$W_{V(Y)} = P^T W_{V(X)}.$$

Thus the walk matrices relative to the set of all vertices in isomorphic graphs are equal up to reordering the rows. If these walk matrices are invertible, no two rows are equal, and therefore the ordering of the vertices obtained from the lexicographic ordering of the rows of W is canonical.

5.5.2 Theorem. *Two controllable graphs are isomorphic if and only their ordered walk matrices are equal.*

Proof. One direction is proved in the paragraph above. For the other direction, note that if their ordered matrices are equal, there is a permutation matrix P so that $W_{V(Y)} = P^T W_{V(X)}$. Then

$$W = \begin{pmatrix}\mathbf{1} & B\mathbf{1} & \dots & B^{n-1}\mathbf{1}\end{pmatrix} = \begin{pmatrix}\mathbf{1} & (P^T AP)\mathbf{1} & \dots & (P^T AP)^{n-1}\mathbf{1}\end{pmatrix}.$$

Thus, because the characteristic polynomials of B and $P^T AP$ have degree n, we also have $B^n\mathbf{1} = (P^T AP)^n\mathbf{1}$. Thus

$$B\begin{pmatrix}\mathbf{1} & B\mathbf{1} & \dots & B^{n-1}\mathbf{1}\end{pmatrix} = (P^T AP)\begin{pmatrix}\mathbf{1} & (P^T AP)\mathbf{1} & \dots & (P^T AP)^{n-1}\mathbf{1}\end{pmatrix},$$

and the result now follows because W is invertible. □

As a consequence of the above lemma, we have a polynomial time isomorphism algorithm for controllable graphs.

5.6 Isomorphism

Let X be a graph on n vertices with adjacency matrix A and let y be a vector in $\mathbb{R}^n$. Let Y be a graph on n vertices with adjacency matrix B and let z be a vector in $\mathbb{R}^n$. We say that the pairs (X, y) and (Y, z) are *isomorphic* if there is an orthogonal matrix L such that

$$LA = BL, \quad \text{and} \quad Ly = z.$$

We will use $W_{X,y}$ to denote the walk matrix of X relative to y. Analogously for $W_{Y,z}$. Note that as a consequence of the isomorphism between (X, y)

and (Y, z), we have $LW_{X,y} = W_{Y,z}$; thus controllability is preserved by isomorphism. Further

$$W_{Y,z}^T W_{Y,z} = W_{X,y}^T L^T L W_{X,y} = W_{X,y}^T W_{X,y}.$$

If the pairs (A, y) and (B, z) are isomorphic, then A and B must have the same characteristic polynomial. Moreover, $W_{Y,z}^T W_{Y,z} = W_{X,y}^T W_{X,y}$ implies that, for all k,

$$y^T A^k y = z^T B^k z,$$

thus giving that

$$y^T (I - tA)^{-1} y = z^t (I - tB)^{-1} z.$$

As it turns out, a converse is also true.

5.6.1 Lemma. *Assume A and B are similar matrices, with spectral decompositions*

$$A = \sum_{r=0}^{d} \theta_r E_r, \qquad B = \sum_{r=0}^{d} \theta_r F_r.$$

Consider vectors y and z. The following are equivalent.

(a) $y^T E_r y = z^T F_r z$, *for all* r.

(b) $y^T (I - tA)^{-1} y = z^T (I - tB)^{-1} z$.

(c) $W_{Y,z}^T W_{Y,z} = W_{X,y}^T W_{X,y}$.

Proof. The equivalence between (a) and (b) follows from Equation (5.3.1). Also, as we have seen, $W_{X,y}^T W_{X,y}$ determines $y^T (I - tA)^{-1} y$, similarly for Y and z, so (c) implies (b).

Now, we assume (a). If Y is the matrix whose columns are $E_r y$ and Z is the matrix whose columns are $F_r z$, we have $Y^T Y = Z^T Z$. On the other hand, if V is the $(d+1) \times (d+1)$ matrix so that $V_{ij} = \theta_i^{j-1}$, then

$$W_{X,y} = YV \quad \text{and} \quad W_{Y,z} = ZV,$$

and therefore

$$W_{X,y}^T W_{X,y} = V^T Y^T Y V = V^T Z^T Z V = W_{Y,z}^T W_{Y,z}. \qquad \square$$

The lemma gives the important consequence below.

5.6.2 Theorem. *Two pairs (A, y) and (B, z) are isomorphic if and only if A and B are similar, and $y^T(I - tA)^{-1}y = z^T(I - tB)^{-1}z$.*

Proof. If (A, y) and (B, z) are isomorphic, then A and B are similar, and $W_{Y,z}^T W_{Y,z} = W_{X,y}^T W_{X,y}$, thus one direction follows from the previous lemma.

Now assume A and B are similar. We must construct an orthogonal matrix L that gives the similarity, and satisfies $Ly = z$.Any orthogonal matrix L' mapping the orthonormal bases of the eigenspaces of A to the bases of the corresponding eigenspaces of B is so that $L'A = BL'$. In choosing a basis for each eigenspace, we can always start with an arbitrarily chosen unit vector, so define L so that $LA = BL$, and, for all r,

$$L\left(\frac{1}{\sqrt{y^T E_r y}} E_r y\right) = \frac{1}{\sqrt{z^T F_r z}} F_r z.$$

As $y^T E_r y = z^T F_r z$ from Lemma 5.6.1, it follows that, for all r, $L(E_r y) = F_r z$. Thus

$$Ly = L \sum_{r=0}^{d} E_r y = \sum_{r=0}^{d} F_r z = z.$$ □

We derive two important consequences.

5.6.3 Corollary. *Pairs (X, S) and (Y, T) are isomorphic if and only if X is cospectral to Y and the cone of X relative to S is cospectral to the cone of Y relative to T.*

Proof. Assuming $A = A(X)$ and $B = A(Y)$ are similar, it follows from Lemma 5.4.4 that $\widehat{X_S}$ and $\widehat{Y_T}$ are cospectral if and only if

$$e_S^T(I - tA)^{-1}e_S = e_T^T(I - tB)^{-1}e_T.$$

From the previous theorem, the result follows. □

From Corollary 4.6.3 it follows that if X and Y are cospectral then $\overline{X}$ and $\overline{Y}$ are cospectral if and only if

$$\mathbf{1}^T(I - tA(X))^{-1}\mathbf{1} = \mathbf{1}^T(I - tA(Y))^{-1}\mathbf{1}.$$

So Theorem 5.6.2 imply the important result of Johnson and Newman [42] that if X and Y are cospectral with cospectral complements, then there is an orthogonal matrix L such that

$$L^T A(X) L = A(Y), \quad L^T(A(\overline{X}))L = A(\overline{Y}).$$

5.7 Isomorphism of Controllable Pairs

Our first result generalizes Lemma 2.4 from [58].

5.7.1 Lemma. *Suppose the pairs (X,S) and (Y,T) are isomorphic and controllable. Then the matrix $W_T W_S^{-1}$ is orthogonal and represents the isomorphism from (X,S) to (Y,T).*

Proof. Let A and B be the adjacency matrices of X and Y respectively.

Since the pairs are isomorphic, $W_S^T W_S = W_T^T W_T$. Since they are controllable, W_S and W_T are invertible and therefore

$$W_T W_S^{-1} = W_T^{-T} W_S^T = (W_T W_S^{-1})^{-T}$$

Hence $Q = W_T W_S^{-1}$ is orthogonal.

Let C denote the companion matrix of $\phi(X,t)$. Then

$$AW_S = W_S C,$$

and, since A and B are similar,

$$BW_T = W_T C.$$

Hence

$$BW_T W_S^{-1} = W_T C W_S^{-1} = W_T W_S^{-1} A$$

and thus $B = QAQ^{-1}$.

Finally, since $QW_S = W_T$, we have $Qe_S = e_T$. □

5.7.2 Corollary. *If the pairs (X,S) and (X,T) are isomorphic and controllable and $Q = W_T W_S^{-1}$, then Q commutes with $A(X)$ and $Q^2 = I$.*

Proof. From the lemma we have $QAQ^{-1} = A$, so Q and A commute. Since the eigenvalues of A are all simple, this implies that Q is a polynomial in A and therefore it is a symmetric matrix. □

When the hypotheses of this corollary hold, the matrix Q can be viewed as a kind of "approximate" automorphism of order two—it is rational, commutes with A and swaps the characteristic vectors of S and T. If S and T are single vertices a and b, then Q will be block diagonal with one block of the form

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and the other an orthogonal matrix of order $(n-2)\times(n-2)$ which commutes with the adjacency matrix of $X \setminus \{a,b\}$.

5.7.3 Lemma. *If (A,y) and (B,z) are controllable and $y^T(I-tA)^{-1}y = z^T(I-tB)^{-1}z$, then (A,y) and (B,z) are isomorphic.*

Proof. This is a combination of Lemma 5.6.1 and Lemma 5.7.1, noting that the latter holds just the same for vectors y and z instead of e_S and e_T. □

5.8 Laplacians

The theory we have presented will hold for any symmetric matrix. If $D = D(X)$ is the diagonal matrix of valencies of the vertices of X and A is its adjacency matrix, recall that $L(X) = D - A$ is the *Laplacian* of X. This is a symmetric matrix, positive semidefinite matrix, with row sums zero.

If $a, b \in V(X)$, define

$$H_{a,b} := (e_a - e_b)(e_a - e_b)^T.$$

If $ab \notin E(X)$, and the graph Y is obtained by adding the edge ab to X, then

$$L(Y) = L(X) + H_{a,b}.$$

Thus

$$L(X) = \sum_{ab \in E(X)} H_{a,b}.$$

Now

$$\begin{aligned}\det(tI - L - H_{a,b}) &= \det[(tI-L)(I-(tI-L)^{-1}H_{a,b})] \\ &= \det(tI-L)\det(I-(tI-L)^{-1}(e_a-e_b)(e_a-e_b)^T) \\ &= \det(tI-L)(1-(e_a-e_b)^T(tI-L)^{-1}(e_a-e_b))\end{aligned}$$

and if $h := e_a - e_b$, then

$$\frac{\phi(L(Y),t)}{\phi(L(X),t)} = 1 - h^T(tI-L)^{-1}h = 1 - \sum_\lambda \frac{h^T F_\lambda h}{t-\lambda}$$

where $L = \sum_\lambda \lambda F_\lambda$ is the spectral decomposition of L. It follows that the eigenvalues of $L(Y)$ are determined by the eigenvalues of $L(X)$ along with the squared lengths of the projections of $e_a - e_b$ onto the eigenspaces of $L(X)$.

If we get Y from X by deleting the edge ab, then we find that

$$\frac{\phi(L(Y),t)}{\phi(L(X),t)} = 1 + \sum_{\lambda} \frac{h^T F_\lambda h}{t-\lambda}$$

We observe that $L^r h$ is orthogonal to $\mathbf{1}$, and so the dimension of the L-module generated by h is at most $n-1$. We say that the pair of vertices $\{a,b\}$ is *controllable* relative to the Laplacian if

$$W = \begin{pmatrix} \mathbf{1} & h & Lh & \dots & L^{n-2}h \end{pmatrix}$$

has rank n.

If $\{a,b\}$ is controllable and P is an automorphism of X that fixes $\{a,b\}$, then either

$$P(e_a - e_b) = e_a - e_b$$

and $PW = W$, or

$$P(e_a - e_b) = e_b - e_a$$

and P acts as multiplication by -1 on the $n-1$-dimensional subspace orthogonal to $\mathbf{1}$. As a consequence, its trace is negative, and so it is not a permutation matrix, and in the former case $P = I$. We conclude that if $\{a,b\}$ is controllable with respect to L, then only the identity automorphism fixes the set $\{a,b\}$.

5.9 Control Theory

In this section we provide a brief introduction to some concepts from control theory. Our favorite source for this material is the book of Kailath [43] (but there is a lot of choice).

Consider a discrete system whose state at time n is x_n, where $x_n \in \mathbb{F}^d$. Assume A is a $d \times d$ matrix, and $b \in \mathbb{F}^d$. The states are related by the recurrence

$$x_{n+1} = Ax_n + u_n b \qquad (n \geq 0). \tag{5.9.1}$$

where $(u_n)_{n\geq 0}$ is an arbitrary sequence of scalars. The output c_n at time n is equal to $c^T x_n$, where c is fixed. The basic problem is determine information about the state of the system given (u_n) and (c_n). From (5.9.1) we find that

$$\sum_{n\geq 0} t^n x_{n+1} = A\sum_{n\geq 0} t^n x_n + \Big(\sum_{n\geq 0} u_n t^n\Big) b.$$

If we define

$$X(t) := \sum_{n\geq 0} t^n x_n, \quad u(t) := \sum_{n\geq 0} u_n t^n, \quad c(t) := \sum_{n\geq 0)} c_n t^n$$

then we may rewrite our recurrence as

$$t^{-1}(X(t) - x_0) = AX(t) + u(t)b,$$

and consequently

$$X(t) = (I - tA)^{-1}x_0 + tu(t)(I - tA)^{-1}b. \tag{5.9.2}$$

Thus we have two distinct contributions to the behaviour of the system: one determined entirely by A and the initial state x_0, the other determined by A, b and $u(t)$. It follows from (5.9.2) that the state of the system is always in the column space of the *controllability matrix*

$$W = \begin{pmatrix} b & Ab & \dots & A^{d-1}b \end{pmatrix}$$

The system is *controllable* if W is invertible.

(Note that our "exposition" of control theory is confined to the simplest case. In general b and c are replaced by matrices B and C. The system is then controllable if the the A-module generated by $\operatorname{col}(B)$ is $\mathbb{F}^v$, and observable if the module generated by $\operatorname{col}(C)$ is $\mathbb{R}^v$. This more general case forced itself on us in our treatment of Laplacians.)

It is convenient to assume $x_0 = 0$. Then we have

$$c(t) = tu(t)\, c^T(I - tA)^{-1}b.$$

If the *observability matrix*

$$\begin{pmatrix} c^T \\ c^T A \\ \vdots \\ c^T A^{d-1} \end{pmatrix}$$

is invertible, then it is possible to infer the state of the system at time m from the observations $c_m, \dots, c_{m+d-1}$. In this case we say that the system is *observable*. Note that the system is observable if and only the pair (A, b) is controllable.

The series

$$c^T(I - tA)^{-1}b,$$

is known as the *transfer function* of the system. In control theory our variable t is normally replaced by a variable z^{-1}; thus the transfer function becomes $c^T(zI - A)^{-1}b$.

Notes

This chapter is based in large part on [36] and [39].

O'Rourke and Touri prove [50] that for random graphs $X = G(n, p)$, the n pairs (A, e_i) for $i \in V(X)$ are all controllable, with probability going to 1 as $n \to \infty$. In [**?**], they prove (in our terms) that almost all graphs are controllable.

In [33] it is proved that controllable graphs are reconstructible. Tutte [] proved that a graph is reconstructible if its characteristic polynomial is irreducible over the rationals.

The results in Section 5.6 extend an important result of Johnson and Newman [42], who essentially proved Theorem 5.6.2 for $y = z = \mathbf{1}$.

Exercises

5-1. Let $C_S(X, t)$ be the generating series for the walks in X that start and finish at a vertex in S, meaning, the coefficient of t^k is the number of walks of length k that start and end at S. Show that entries of $W_S^T W_S$ suffice to determine $C_S(X, t)$.

5-2. If $z \in \mathbb{R}^n$, then the *minimal polynomial* of A relative to z is the monic polynomial p of least degree such that $p(A)z = 0$. If ψ is the usual minimal polynomial of A, show that p divides ψ.

5-3. Show that the degree of the minimal polynomial of A relative to x_S equals $\operatorname{rk}(W_S)$.

5-4. Show that the dual degree of a is zero if and only if a is an isolated vertex. Show that the dual degree of a is one if and only if X is a cone at a over a regular graph. Try to characterize the graphs so that a vertex has the dual degree equal to two.

5-5. Prove in detail that if X and Y are cospectral with cospectral complements, then there is an orthogonal matrix L so that $LA(X) = A(Y)L$, and $LA(\overline{X}) = A(\overline{Y})L$.

Chapter 6

Cospectral Vertices

In Chapter 4, we developed a theory that relates walks in graphs and the spectrum. For instance, we saw in Theorem 4.10 that two vertices a and b are cospectral if and only $W_{a,a}(X,t) = W_{b,b}(X,t)$. The connection with quantum walks is our motivation—as we know, if we have perfect state transfer on X, then the vertices a and b are cospectral. In Chapter 5 we focused on the walk modules, and derived fundamental properties.

In this chapter, we intend to apply the theory built in the previous chapters to quantum walks.

6.1 Walk modules of cospectral vertices

Walk modules provide a yet another way of characterizing cospectral vertices.

6.1.1 Theorem. *The following are equivalent.*

(a) Vertices a and b are cospectral in the graph X.

(b) The A-modules generated by $e_a + e_b$ and $e_a - e_b$ are orthogonal.

(c) The A-modules generated by e_a and e_b are isomorphic, and this isomorphism is given by a symmetric matrix Q that commutes with A, interchanges e_a and e_b, and satisfies $Q^2 = I$.

Proof. As usual, let $A = \sum_{r=0}^{d} \theta_r E_r$ be the spectral decomposition of $A = A(X)$.

For any projection E_r, we have

$$(E_r(e_a+e_b))^T E_r(e_a-e_b) = (e_a+e_b)^T E_r(e_a-e_b) = (E_r)_{a,a} - (E_r)_{b,b}.$$

Moreover, $(E_s(e_a+e_b))^T E_r(e_a-e_b) = 0$ whenever $s \neq r$. Thus, the A-modules generated by e_a+e_b and e_a-e_b are orthogonal if and only if $(E_r)_{a,a} = (E_r)_{b,b}$ for each eigenvalue θ_r of X.

Now observe that $\mathbb{R}^n$ can be decomposed into three orthogonal subspaces: the A-module generated by (e_a+e_b), call it W_+, the one generated by (e_a-e_b), say W_-, and the orthogonal complement of their direct sum, denoted by W_0. Define the map Q that acts as the identity in W_+ and in W_0, and multiplies vectors in W_- by -1. It is an isomorphism of $\mathbb{R}^n$ that interchanges the A-modules generated by e_a and e_b. Moreover, $Q^2 = I$, its eigenspaces are orthogonal, and each of them is A-invariant. Thus Q is symmetric and commutes with A.

If (c) holds, then, for all r, recalling that E_r is a polynomial in A, we have

$$e_a^T E_r e_a = e_a^T E_r Q Q E_r e_a = (QE_r e_a)^T (QE_r e_a) = (E_r Q e_a)^T (E_r Q e_a) = e_b^T E_r e_b.$$

□

The theorem implies that, if a and b are cospectral and z lies in the A-module generated by e_a+e_b, then $z_a = z_b$. If a (or b) is controllable, then $\mathbb{R}^n$ is the direct sum of the modules generated by e_a+e_b and e_a-e_b.

6.2 Characterizing Cospectral Vertices

There is a surprising number of interesting ways to characterize pairs of cospectral vertices. We compile a list below, based on Theorems 4.3.2 and 6.1.1, and Lemma 5.6.1.

6.2.1 Theorem. *Let a and b be vertices in X. Then the following statements are equivalent:*

(a) a and b are cospectral, that is, for all r, $(E_r)_{a,a} = (E_r)_{b,b}$.

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

(c) If W_a and W_b are the walk matrices for a and b respectively, then $W_a^T W_a = W_b^T W_b$.

(d) *The* $\mathbb{R}[A]$*-modules generated by* $e_a - e_b$ *and* $e_a + e_b$ *are orthogonal.*

(e) *There is a symmetric matrix* Q*, with* $Q^2 = I$ *and so that* $AQ = QA$*, satisfying* $Qe_a = e_b$*.*

(f) $W_{a,a}(X,t) = W_{b,b}(X,t)$*.*

(g) *For all integers* k*,* $(A^k)_{a,a} = (A^k)_{b,b}$*.* □

6.3 Walk-Regular Graphs

A graph is *walk-regular* if all vertices in it are cospectral, or, equivalently, if each matrix in the algebra generated by $A(X)$ has constant diagonal. Any vertex-transitive graph is walk regular. However the graph in Figure 6.1 is walk regular but not vertex transitive. (As it happens, it is cospectral to the line graph of the cube, which is vertex transitive.)

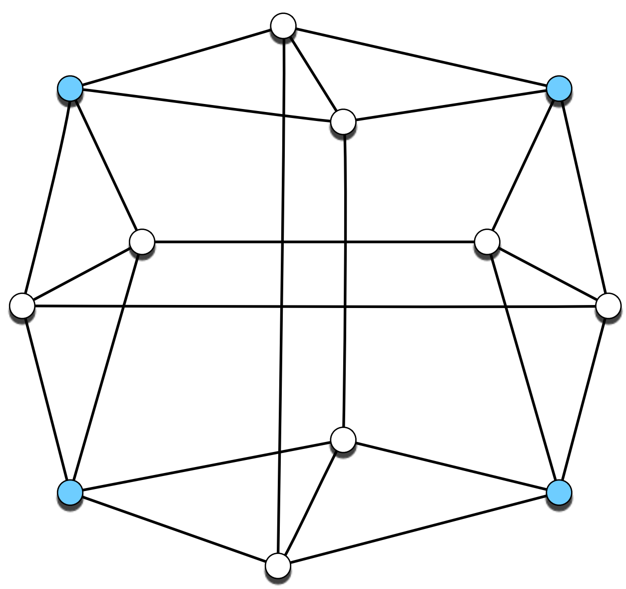

Figure 6.1: A Walk-Regular Graph that is not vertex transitive.

The complement of a walk-regular graph is walk regular. Our next result is from Van Dam [56]).

6.3.1 Lemma. *If X is connected and regular and has at most four distinct eigenvalues, it is walk regular.*

Proof. If A is connected and regular on n vertices, then $\frac{1}{n}J$ is one of its spectral idempotents. If θ_1, θ_2, θ_3 are the eigenvalues of A distinct from the valency of X and

$$p(t) = (t - \theta_1)(t - \theta_2)(t - \theta_3),$$

then $p(A)$ is a multiple of J. This implies that A^3 is a linear combination of J, I, A and A^2 and hence that the diagonal of A^3 is constant. Since the minimal polynomial of A has degree at most four, it follows that if $k \geq 4$ then A^k is a linear combination of A^r for $r = 0, \ldots, 3$ and therefore its diagonal is constant. □

You might prove that a connected regular bipartite graph with at most five distinct eigenvalues is walk regular.

6.3.2 Theorem. *If X is walk regular and $|V(X)| \geq 3$, then the number of simple eigenvalues of X is at most $|V(X)|/2$.*

Proof. Assume X is as given and $n = |V(X)|$. If X is not connected then each component is walk regular with the same characteristic polynomial and the result holds because there are no simple eigenvalues. Hence assume X is connected and its valency, say k, is a simple eigenvalue.

Suppose X has a second simple eigenvalue λ, with eigenvector z. Then the idempotent E_λ is a non zero scalar multiple of zz^T. Since all diagonal entries of E_λ are equal, all entries of z have the same absolute value. We may assume z is a ±1-vector. Since $\lambda \neq k$ the eigenvectors $\mathbf{1}$ and z are orthogonal and hence z must contain an equal number of 1's and -1's. This implies that n is even. We can also see that $k - \lambda$ must be even.

Assume that X has exactly s simple eigenvalues. If the eigenvalues of X are

$$k = \theta_1 \geq \cdots \geq \theta_n$$

then the eigenvalues of $\overline{X}$ are

$$n - 1 - k \geq -\theta_n - 1 \geq \cdots \geq -\theta_2 - 1.$$

Since $\overline{X}$ is walk-regular, if it is not connected then it has no simple eigenvalues and X has at most two simple eigenvalues. If $\overline{X}$ is connected then its valency $n-1-k$ is a simple eigenvalue and so $\overline{X}$ has exactly s simple eigenvalues. Now the simple eigenvalues of X lie in the set

$$k, k-2, \ldots, -k$$

and so $s \leq k+1$ and, applying the same argument to $\overline{X}$ yields $s \leq n-k$. Therefore $2s \leq n+1$. As n is even, the result follows. □

It can be shown that if the number of simple eigenvalues of a walk regular graph X on more than two vertices is greater than two, then $|V(X)|$ is divisible by four.

6.4 State Transfer on Walk-Regular Graphs

In this section, we see an application of the concept of walk regular graphs to quantum walks.

6.4.1 Lemma. *If X is walk regular and perfect state transfer occurs on X, then $|V(X)|$ must be even.*

Proof. Suppose perfect state transfer takes place from a to b at time τ. Then there is a complex number γ where $|\gamma| = 1$ such that

$$U(\tau)_{a,b} = U(\tau)_{b,a} = \gamma.$$

As $|\gamma| = 1$, we see that $U(\tau)_{a,a} = 0$ and, as X is walk-regular, all diagonal entries of $U(\tau)$ are zero and in particular, $\operatorname{tr}(U(\tau)) = 0$. Since

$$U(2\tau)_{a,a} = \gamma^2$$

we also see that that $U(2\tau) = \gamma^2 I$. We conclude that the eigenvalues of $U(\tau)$ are all $\pm\gamma$ and, since $\operatorname{tr}(U(\tau)) = 0$, both γ and $-\gamma$ have multiplicity $|V(X)|/2$. □

If m_r denotes the multiplicity of the eigenvalue θ_r, then

$$\operatorname{tr}(U(t)) = \sum_{r=0}^{d} m_r \exp(\mathrm{i}t\theta_r).$$

If X has integer eigenvalues only, we may define the Laurent polynomial $\mu(z)$ by

$$\mu(z) := \sum_{r=0}^{d} m_r z^{\theta_r}.$$

We call $\mu(z)$ the *multiplicity enumerator* of X.

6.4.2 Lemma. *Let X be a walk-regular graph with integer eigenvalues. If perfect state transfer occurs on X, then $\mu(z)$ has a zero on the unit circle of the complex plane.*

Proof. The trace of $U(t)$ is zero if and only if $\mu(\mathrm{e}^{\mathrm{i}t}) = 0$. □

The characteristic polynomial of the graph in Figure 6.1 is

$$(t-4)(t-2)^3 t^3 (t+2)^5$$

and its multiplicity enumerator is

$$\mu(z) = z^{-2}(z^6 + 3z^4 + 3z^2 + 5).$$

This polynomial has no roots on the unit circle, and we conclude that perfect state transfer does not occur in that graph.

We see no reason to believe that, if perfect state transfer occurs on a walk-regular graph at time τ, then $U(\tau)$ must be a multiple of a permutation matrix. (But we do not have an example where it is not.)

For more information on walk-regular graphs, see [32]. The computations in this section were carried out in sage [54]. Van Dam [56] studies regular graphs with four eigenvalues, as we noted these provide examples of walk-regular graphs.

6.5 Parallel Vertices

We say that two vertices a and b of X are *parallel* if for each r, the projections $E_r e_a$ and $E_r e_b$ are parallel. We will see that this relation arises naturally in our work on state transfer and other phenomena. If all eigenvalues of X are simple, then any two vertices are parallel, hence there is no shortage of examples.

To begin, we show that the concept has some combinatorial significance.

6.5.1 Lemma. *Suppose a and b are parallel vertices in X with the same eigenvalue support. If π is an equitable partition of X and $\{a\}$ is a singleton cell in π, then so is $\{b\}$.*

Proof. Let π be an equitable partition with normalized characteristic matrix Q. Then $\{a\}$ is a cell of π if and only if $QQ^T e_a = e_a$. Since QQ^T commutes with any polynomial in A, we have

$$E_r e_a = E_r QQ^T e_a = QQ^T E_r e_a.$$

As a and b have the same eigenvalue support, if $E_r e_a \neq 0$, then $E_r e_b \neq 0$. Further, since a and b are parallel, it follows that e_b lies in the span of the vectors $E_r e_a$. Therefore $QQ^T e_b = e_b$ and so $\{b\}$ is a cell of π. □

Of course this result implies that if a and b have the same eigenvalue support and are parallel, then $\mathrm{Aut}(X)_a = \mathrm{Aut}(X)_b$.

6.5.2 Lemma. *Distinct vertices a and b of X are parallel if and only if all poles of the rational function $\phi(X \setminus \{a,b\}, t)/\phi(X,t)$ are simple.*

Proof. By Corollary 4.5.2, if $D = \{a,b\}$ then the multiplicity of the pole at θ_r in $\phi(X \setminus D, t)/\phi(X,t)$ is equal to $\mathrm{rk}((E_r)_{D,D})$. We have

$$|(E_r)_{a,b}|^2 = (e_a^T E_r e_b)^2 = \langle E_r e_a, E_r e_b \rangle^2 \leq \|E_r e_a\|^2 \|E_r e_b\|^2 = (E_r)_{a,a}(E_r)_{b,b}$$

whence it follows that $\mathrm{rk}((E_r)_{D,D}) = 1$ if and only if a and b are parallel. □

6.5.3 Lemma. *The walk modules relative to vertices a and b of X are equal if and only if a and b are parallel and have the same eigenvalue support.*

Proof. Each element of W_a can be expressed as $p(A)e_a$ for some polynomial p. As $E_r p(A) e_a = p(\theta_r) E_r e_a$, we see that the vectors $E_r e_a$ form an orthogonal basis for $\mathrm{col}\, W_a$ and the intersection of W_a with any eigenspace of A has dimension at most one.

If $W_a = W_b$ then $E_r W_a = E_r W_b$, but $E_r W_a$ and $E_r W_b$ are spanned respectively by $E_r e_a$ and $E_r e_b$. Therefore a and b are parallel and have the same eigenvalue support. For the converse, if a and b are parallel and have the same eigenvalue support then $E_r e_a$ and $E_r e_b$ span the same space for each r, and thus $W_a = W_b$. □

6.6 Strongly Cospectral Vertices

Recall that we define vertices a and b in X to be strongly cospectral if, for each idempotent E_r,

$$E_r e_a = \pm E_r e_b.$$

We immediately have the following:

6.6.1 Lemma. *Two vertices a and b in X are strongly cospectral if and only if they are parallel and cospectral.* □

Taking note of Lemma 6.5.3, we have a second useful characterization.

6.6.2 Corollary. *Let a and b be vertices in X with walk matrices W_a and W_b respectively. Then a and b are strongly cospectral if and only if they are cospectral and* $\operatorname{col}(W_a) = \operatorname{col}(W_b)$. □

If a and b are vertices in X, we say an element f in $\mathbb{R}^{V(X)}$ is *balanced* if $f(a) = f(b)$ and is *skew* if $f(a) = -f(b)$. A subspace is balanced or skew if each vector in it is balanced or, respectively, skew.

6.6.3 Lemma. *Two vertices a and b in X are strongly cospectral if and only if each eigenspace is balanced or skew relative to the vertices a and b.*

Proof. If a and b are strongly cospectral, then either $E_r(e_a - e_b) = 0$ or $E_r(e_a + e_b) = 0$. Since $\operatorname{col}(E_r)$ is the θ_r-eigenspace, it follows that either each eigenvector in the θ_r-eigenspace is balanced, or each eigenspace is skew. The converse follows easily. □

Since cospectral vertices necessarily have the same eigenvalue support, we have:

6.6.4 Corollary. *If the eigenvalues of X are simple, then cospectral vertices are strongly cospectral.* □

Suppose X is arc regular (i.e., X is walk regular and the walk generating functions $W_{a,b}(X,t)$ are equal for all arcs (a,b)). Assume the valency of X is k. If $b_1 \sim a$ and $\theta \neq \pm k$, then

$$\theta(E_\theta)_{a,a} = \sum_{b\sim a}(E_\theta)_{a,b} = k(E_\theta)_{a,b_1}$$

Since $|\theta| < k$, adjacent vertices cannot be strongly cospectral, and so we deduce that we cannot get perfect state transfer from a vertex to its neighbour in an arc-transitive graph. A variant of this argument shows that in a distance-regular graph, strongly cospectral vertices are antipodal. More on that in Chapter 14.

6.6.5 Lemma. *If all vertices in X are strongly cospectral, then $X = K_2$.*

Proof. If all vertices of X are strongly cospectral to a, then the θ_r-eigenspace of X is spanned by $E_r e_a$, and therefore all eigenvalues of X are simple. If all vertices are cospectral, then X is walk regular and therefore by Theorem 6.3.2 we deduce that $|V(X)| \leq 2$. □

6.6.6 Lemma. *The number of vertices strongly cospectral to a is bounded above by the size of the eigenvalue support of a.*

Proof. If vertices a and b are strongly cospectral, then e_b is a signed sum of the nonzero vectors $E_r e_a$, say

$$e_b = \sum_{r=0}^{d} \sigma_r(b) E_r e_a,$$

where $\sigma_r(b) = \pm 1$ and the sum is over the nonzero vectors $E_r e_a$. Let S be the matrix with rows indexed by the vertices strongly cospectral to a and columns by the indices r such that $E_r e_a \neq 0$, and with br-entry equal to $\sigma_r(b)$. If M is the matrix with the non-zero vectors $E_r e_a$ as columns, then

$$\begin{pmatrix} I \\ 0 \end{pmatrix} = MS.$$

Therefore the rows of S are linearly independent and the claim follows. □

6.7 Examples of Strongly Cospectral Vertices

We present some examples of strongly cospectral vertices.

6.7.1 Theorem. *Let X be the graph obtained from vertex-disjoint graphs Y and Z by joining a vertex a in Y to a vertex b in Z by a path P of length at least one. If a and b are cospectral in X, they are strongly cospectral.*

Proof. Assume $A = A(X)$ and, recall, $\phi_{a,b}(X,t)$ denotes $[\operatorname{adj}(tI - A)]_{a,b}$. From the spectral decomposition of A, we have

$$\frac{\phi_{a,b}(X,t)}{\phi(X,t)} = ((tI - A)^{-1})_{a,b} = \sum_{r=0}^{d} \frac{(E_r)_{a,b}}{t - \theta_r},$$

showing that the poles of $\phi_{a,b}(X,t)/\phi(X,t)$ are simple. From Corollary 4.4.4, we have

$$\phi_{a,b}(X,t) = \sum_{P \in \mathcal{P}_{a,b}} \phi(X \setminus P, t),$$

where the sum is over all paths in X that join a to b. By construction there is only one path in X that joins a to b, and therefore

$$\phi_{a,b}(X,t) = \phi(Y \setminus a, t)\phi(Z \setminus b, t).$$

If Q is the path we get from P by deleting its end-vertices.

$$\frac{\phi(X \setminus \{a,b\}, t)}{\phi(X,t)} = \phi(Q,t)\frac{\phi(Y \setminus a, t)\phi(Z \setminus b, t)}{\phi(X,t)} = \phi(Q,t)\frac{\phi_{a,b}(X,t)}{\phi(X,t)}$$

We conclude that the poles of $\phi(X \setminus \{a,b\}, t)/\phi(X,t)$ are all simple and so, by Lemma 6.5.2, it follows that a and b are strongly cospectral. □

Note that a and b will be cospectral in X if Y and Z are cospectral and also $Y \setminus a$ and $Z \setminus b$ are cospectral.

Now we consider a rabbit-ear construction. Recall that we use $\mathrm{mult}(\lambda, X)$ to denote the multiplicity of λ as an eigenvalue of X.

6.7.2 Lemma. *Let a be a vertex in X and let Z be formed from X by joining two new vertices of valency one to a. If $\mathrm{mult}(0, X \setminus a) \le \mathrm{mult}(0, X)$, the two new vertices are strongly cospectral in Z.*

Proof. The two new vertices are swapped by an automorphism of Z, and so they are cospectral. Applying Lemma 4.7.1 twice, we find that

$$\phi(Z,t) = t^2\phi(X,t) - 2t\phi(X \setminus a, t),$$

and so, by Lemma 6.5.2, we can prove the result by verifying that the poles of

$$\frac{\phi(X,t)}{t(t\phi(X,t) - 2\phi(X \setminus a, t))}$$

are simple. Now

$$\frac{\phi(X,t)}{(t\phi(X,t) - 2\phi(X \setminus a, t))} = \frac{1}{t - 2\frac{\phi(X \setminus a, t)}{\phi(X,t)}}$$

and, by Equation (4.3.4), the poles of the above rational function are simple.

So the lemma is proved if we show that 0 is not a zero of

$$t - 2\frac{\phi(X \setminus a, t)}{\phi(X,t)},$$

equivalently, not a zero of the rational function

$$\frac{\phi(X \setminus a, t)}{\phi(X, t)}.$$

This holds if and only if $\mathrm{mult}(0, X \setminus a) \leq \mathrm{mult}(0, X)$. □

As a sanity check, if $X = K_1$, then $\mathrm{mult}(0, X) = 1$ and $\mathrm{mult}(0, X \setminus a) = 0$ and it follows that the vertices of valency one in P_3 are strongly cospectral. (This is very likely the most complicated proof of this fact we can provide.)

6.8 Characterizing Strongly Cospectral Vertices

Our terminology is somewhat tongue-in-cheek: a *symmetry* of a graph is an orthogonal matrix which commutes with its adjacency matrix. As we have already seen, cospectrality between vertices a and b is characterized by the existence of a symmetric symmetry that interchanges a and b. It turns out strong cospctrality can also be characterized in terms of symmetries.

6.8.1 Lemma. *The vertices a and b in X are strongly cospectral if and only if there is an orthogonal matrix Q such that:*

(a) Q is a polynomial in A, and, additionally, it is a rational matrix.

(b) $Qe_a = e_b$.

(c) $Q^2 = I$.

Proof. As usual, the spectral decomposition of A is given by $A = \sum_{r=0}^{d} \theta_r E_r$. There are $\sigma_r \in \{\pm 1\}$ so that, for $E_r e_a = \sigma_r E_r e_b$ if, and only if, the polynomial defined by $p(\theta_r) = \sigma_r$ satisfies $p(A)e_a = e_b$. Moreover, $p(A)^2 = I$ if and only if $p(\theta_r) = \pm 1$.

So the only thing remaining to show is that $p(A)$, defined as above, is a rational matrix. We will use some basic facts about field extensions, which we will revisit in Chapter 7.

Let $\mathbb{E}$ be the extension of the rationals obtained by adjoining the eigenvalues of X and let α be an automorphism of $\mathbb{E}$. Assume a and b are strongly cospectral. Then E_r^α, given by applying α to each entry of E_r, is an idempotent in the spectral decomposition of A, associated to the eigenvalue θ_r^α. Therefore $((E_r)_{a,a})^\alpha > 0$ and consequently $((E_r)_{a,b})$ and $((E_r)_{a,b})^\alpha$ must have the same sign. It follows that $Q = p(A)$ is fixed by all field automorphisms of $\mathbb{E}$ and therefore it is a rational matrix. □

We can now provide a compiled list of equivalent characterizations of strongly cospectral vertices, using Theorem 6.2.1, Lemma 6.5.2, Lemma 6.6.1, Lemma 6.5.3, Corollary 6.6.2, and Lemma 6.8.1.

6.8.2 Theorem. *Let a and b be vertices in X. Then the following statements are equivalent:*

(a) a and b are strongly cospectral, that is, for all r, $E_r e_a = \pm E_r e_b$.

(b) $\phi(X \setminus a, t) = \phi(X \setminus b, t)$, and the poles of the rational function $\phi(X \setminus \{a, b\}, t)/\phi(X, t)$ are simple.

(c) If W_a and W_b are the walk matrices for a and b respectively, then $W_a^T W_a = W_b^T W_b$, and $\mathrm{col}(W_a) = \mathrm{col}(W_b)$

(d) The $\mathbb{R}[A]$-modules generated by $e_a - e_b$ and $e_a + e_b$ are orthogonal, a nd their direct sum is equal to the $\mathbb{R}[A]$-module generated by e_a.

(e) There is a symmetric matrix Q, with $Q^2 = I$ and so that Q is a polynomial in A, satisfying $Qe_a = e_b$. □

We leave it as a research problem to find the analogous conditions to conditions (f) and (g) of Theorem 6.2.1.

We saw that if a and b are controllable, then the eigenvalues of X are simple, and so if a and b are controllable and cospectral there is a symmetric orthogonal matrix Q which commutes with A and maps e_a to e_b. In this case we have an explicit expression for Q.

6.8.3 Lemma. *Let a and b be vertices in X with respective walk matrices W_a and W_b. If a and b are controllable and $Q := W_b W_a^{-1}$ then Q is a polynomial in A. Further Q is orthogonal if and only if a and b are cospectral.*

Proof. Let C_ϕ denote the companion matrix of the characteristic polynomial of A. Then

$$AW_a = W_a C_\phi$$

for any vertex a in X. Hence if a and b are controllable,

$$W_a^{-1} A W_a = W_b^{-1} A W_b$$

and from this we get that

$$A W_b W_a^{-1} = W_b W_a^{-1} A.$$

Since X has a controllable vertex its eigenvalues are all simple, and so any matrix that commutes with A is a polynomial in A. This proves the first claim.

From the discussion in Section 5.1, the vertices a and b are cospectral if and only if $W_a^T W_a = W_b^T W_b$, which is equivalent to

$$Q^{-T} = W_b^{-T} W_a^T = W_b W_a^{-1} = Q. \qquad \square$$

6.9 Matrix Algebras

We obtain another view of the results in this chapter by considering the matrix algebra generated by A and xx^T, for some vector x. We will denote this algebra by $\langle A, xx^T \rangle$. This algebra is closed under transpose (and hence is semisimple.)

6.9.1 Lemma. *If the vertices a and b are parallel with the same eigenvalue support, then $\langle A, e_a e_a^T \rangle = \langle A, e_b e_b^T \rangle$.*

Proof. We note that

$$(A^k xx^T A^\ell)(A^m xx^T A^n) = x^T A^{\ell+m} x \, A^k xx^T A^m$$

and it follows the matrices

$$A^k xx^T A^\ell,$$

together with the powers of A, generate $\langle A, xx^T \rangle$. It follows that if $E_0, \ldots, E_d$ are the spectral idempotents of A, then these idempotents together with the (nonzero) matrices $E_r xx^T E_s$ generate $\langle A, xx^T \rangle$.

If a and b are parallel with the same eigenvalue support, then either $E_r e_a e_a^T E_s$ and $E_r e_a e_a^T E_s$ are both zero, or each is a scalar multiple of the other. Hence $\langle A, e_a e_a^T \rangle = \langle A, e_b e_b^T \rangle$. $\square$

The *commutant* of a set S of $n \times n$ matrices is the set

$$\{M \in \mathrm{Mat}_{n\times n}(\mathbb{C}) : MS = SM\}.$$

6.9.2 Corollary. *Assume a and b are parallel vertices in X and with the same eigenvalue support. If the orthogonal matrix Q commutes with A and $Qe_a = e_a$, then $Qe_b = e_b$.*

Proof. The hypotheses simply imply that Q lies in the commutant of $\langle A, e_a e_a^T \rangle$. □

The permutation matrices in the commutant of $\{A, e_a e_a^T\}$ form the subgroup $\mathrm{Aut}(X)_a$ of $\mathrm{Aut}(X)$. Hence the previous lemma provides another proof that if a and b are strongly cospectral then $\mathrm{Aut}(X)_a = \mathrm{Aut}(X)_b$.

Notes

References to Godsil's early papers and Godsil and Smith. Exers below following from FR paper.

Add reference to Cox (section char. strong cospec vts).

Exercises

6-1. Prove in detail that two vertices a and b in X are strongly cospectral if and only if they are parallel and cospectral.

6-2. Let X be a graph with simple eigenvalues and assume a and b are strongly cospectral vertices. Let $\mathcal{Q}$ be the set of all orthogonal matrices that commute with $A(X)$, that swap a and b or fix both of them, and that are involutions. Let m be the size of the eigenvalue support of a and b. Prove that $\mathcal{Q}$ is a group of order 2^{n-m+1}. Explain why this could fail if X has an eigenvalue which is not simple.

6-3. Let a be a vertex in the graph X and let b be a vertex in Y. If X and Y are cospectral and $X \setminus a$ and $Y \setminus b$ are cospectral, prove that there is an orthogonal matrix Q such that $Q^{-1}A(Y)Q = A(X)$ and $Qe_a = e_b$.

6-4. Prove that a connected regular bipartite graph with at most five distinct eigenvalues is walk regular.

6-5. Define two vertices to be *not-so-strongly cospectral* if they are parallel and have the same eigenvalue support. Show that the number of vertices not-so-strongly cospectral to a is bounded above by the size of the eigenvalue support of a.

6-6. Show that if the number of simple eigenvalues of a walk-regular on more than 2 vertices is greater than 2, then $|V(X)|$ is divisible by four.

6-7. Assume the graph X is connected, with $A = A(X)$, and a and b two of its vertices. Consider the $\mathbb{R}[A]$-module M generated by e_a and e_b. Assume that M is the direct sum of two non-trivial A-invariant submodules, each generated by a linear combination of e_a and e_b. Prove that there exists real numbers p and q, both non-zero, so that, for all E_r,

$$(E_r)_{a,a} - (E_r)_{b,b} = \left(\frac{p}{q} - \frac{q}{p}\right)(E_r)_{a,b}.$$

For a bonus point, adapt the remaining conditions of Theorem 6.2.1 to this situation.

6-8. With the same hypotheses of the exercise above, prove that if a is adjacent to b, or if X is regular, or if a and b have the same degree and are at distance 2, then $p^2 = q^2$.

6-9. Show that if X is regular and its complement is connected, and if a and b are strongly cospectral in X, then they are strongly cospectral in $\overline{X}$.

Part III

State Transfer and Periodicity

Chapter 7

State transfer

Much of the work in connecting algebraic graph theory and quantum walks was motivated by the study of perfect state transfer. In Section **??**, we introduced a Hamiltonian H_{xy}, and verified that it is block diagonal—the block corresponding to the subspace spanned by f_S with $S \subseteq V(X)$ and $|S| = 1$ is the adjacency matrix of the underlying graph. Upon initializing the system in a state given by $f_{\{a\}}$ for some $a \in V(X)$, perfect state transfer means that after some time the state of the system will be $f_{\{b\}}$ for some $b \neq a$. The block decomposition of H_{xy} and Schrödinger's equation imply that the dynamics is given by $U(t) = \exp(\mathrm{i}tA)$, and, as we have already seen in Section 1.3, perfect state transfer is equivalent to having $|U(t)_{a,b}| = 1$ for some t. The goal of this chapter is to study this phenomenon in depth.

To start this chapter we derive a chain of inequalities, starting with

$$|U(t)_{a,b}| \leq \sum_{r=0}^{d} |(E_r)_{a,b}|.$$

Using this we provide an alternate proof that if we have perfect state transfer from a to b, then a and b must be strongly cospectral. This will also lead us to understand certain rationality and parity conditions that the eigenvalues in the eigenvalue support of a must satisfy.

In the remainder of the chapter we develop some of the consequences of these results, in particular we can show that that only finitely many connected graphs with maximum valency at most k admit perfect state transfer.

7.1 Three Inequalities

We derive three inequalities for $|U(t)_{a,b}|$, from which our results follow. We note that in this section, we assume only that A is symmetric and real. Hence our results will also apply to Laplacians or weighted adjacency matrices.

We have

$$U(t)_{a,b} = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} (E_r)_{a,b}$$

and we get the chain of inequalities

$$\begin{aligned} |U(t)_{a,b}| &\leq \sum_{r=0}^{d} |(E_r)_{a,b}| && (7.1.1) \\ &\leq \sum_{r=0}^{d} \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}} && (7.1.2) \\ &\leq \sqrt{\sum_r (E_r)_{a,a} \sum_r (E_r)_{b,b}} && (7.1.3) \\ &= 1. \end{aligned}$$

We aim to develop a better understanding of these three inequalities, starting with (7.1.1). Let σ_r denote the sign of $(E_r)_{a,b}$. (Its value when $(E_r)_{a,b} = 0$ will be irrelevant, we follow custom and take it to be zero.)

7.1.1 Lemma. *We have $|U(t)_{a,b}| \leq \sum_r |(E_r)_{a,b}|$. Equality holds if and only if there is a complex number γ such that $e^{it\theta_r} = \gamma\sigma_r$ whenever $(E_r)_{a,b} \neq 0$.*

Proof. We have

$$U(t)_{a,b} = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} (E_r)_{a,b}$$

Taking absolute values and applying the triangle inequality, the inequality (7.1.1) follows, and equality holds if and only if the stated condition holds. □

If $a \in V(X)$, the numbers $(E_r)_{a,a}$ are nonnegative and sum to 1. Hence they determine a probability density on the eigenvalues of A (whose actual support is the eigenvalue support of a). We call it the *spectral density* of X relative to a. Two vertices have the same spectral density if and only if they are cospectral. If (p_r) and (q_r) are two probability densities with the same finite support, their *fidelity* is defined to be

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

By Cauchy-Schwarz, the fidelity of the densities lies in the interval $[0, 1]$, and it is equal to 1 if and only if the two densities are equal.

7.1.2 Lemma. *The fidelity of the spectral densities of vertices a and b in X is bounded below by $\sum_r |(E_r)_{a,b}|$. Equality holds if and only if a and b are parallel.*

Proof. In (7.1.2), if a and b are vertices in X then by Cauchy-Schwarz

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

and equality holds if and only if $E_r e_a$ and $E_r e_b$ are parallel. □

7.1.3 Lemma. *The fidelity of the spectral densities of vertices a and b in X is bounded above by $\sqrt{\sum_r (E_r)_{a,a} \sum_r (E_r)_{b,b}}$. Equality holds if and only if a and b are cospectral.*

Proof. In (7.1.3), Cauchy-Schwarz applied to the vectors $((\sqrt{(E_r)_{a,a}})_r)$ and $((\sqrt{(E_r)_{b,b}})_r)$, with $r = 0, ..., d$, gives

$$\sum_{r=0}^{d} \sqrt{(E_r)_{a,a}} \sqrt{(E_r)_{b,b}} \leq \sqrt{\sum_{r=0}^{d} (E_r)_{a,a}} \sqrt{\sum_{r=0}^{d} (E_r)_{b,b}}$$

and equality holds if and only if $(E_r)_{a,a} = (E_r)_{b,b}$ for all r, that is, if a and b are cospectral. □

We have already studied cospectral and parallel vertices in the previous chapters. So in order to complete our understanding of perfect state transfer, we will devote some attention to the condition in Lemma 7.1.1 that says that there must be a complex number γ such that $e^{it\theta_r} = \gamma\sigma_r$ whenever $(E_r)_{a,b} \neq 0$. This will be a main topic in this Chapter. However, in the next section we explore another connection between quantum walks and cospectrality.

7.2 Near Enough: Cospectrality

If the initial state of the system is represented by the unit vector e_a, then its state at time t is given by $U(t)e_a$. We can however use density matrices to represent these states instead, as we did in Chapter 2. It will be convenient to use the notation $D_a = e_a e_a^T$ for the *density matrix of* a, and

$$D_a(t) = U(t)D_aU(-t),$$

to represent the density matrix of the state obtained after the evolution.

We prove that if the orbits under $U(t)$ of D_a^T and D_b^T are close enough, then a and b must be cospectral.

Recall from Chapter 5 that the *walk matrix* of X relative to x is the $n \times n$ matrix with columns

$$x, Ax, \ldots, A^{n-1}x.$$

When $x = e_a$, we will use W_a to denote the walk matrix of X relative to a. The non-zero vectors $E_r e_a$ form an orthogonal basis for $\operatorname{col}(W_a)$, thus $\operatorname{rk}(W_a)$ is equal to the size of the eigenvalue support of a.

7.2.1 Lemma. *Let $n = V(X)$ and let ρ be the largest eigenvalue of A. If there is a time t such that*

$$\|D_a(t) - D_b\| < \frac{7}{8n^2\rho^{4n}}.$$

then a and b are cospectral.

Proof. Our first step is to relate $\|D_a(t) - D_b\|$ to $|U(t)_{a,b}|$. Thus,

$$\begin{aligned}
\|D_a(t) - D_b\|^2 &= \operatorname{tr}((D_a(t) - D_b)^2) \\
&= \operatorname{tr}(D_a(t) + D_b - D_a(t)D_b - D_bD_a(t)) \\
&= 2 - 2\langle D_a(t), D_b\rangle
\end{aligned}$$

and, since $\overline{U(t)} = U(-t)$ and since $U(t)$ (along with A) is symmetric,

$$\begin{aligned}
\langle D_a(t), D_b\rangle &= \operatorname{tr}(U(t)e_ae_a^TU(-t)e_be_b^T) \\
&= e_b^TU(t)e_a\, e_a^T\overline{U(t)}e_b \\
&= |U(t)_{a,b}|^2.
\end{aligned}$$

As a rough summary, $\|D_a(t) - D_b\|$ is small if and only if $|U(t)_{a,b}|$ is close to 1. It is an immediate consequence of the inequalities (7.1.1), (7.1.2) and (7.1.3) that if $|U(t)_{a,b}|^2$ gets arbitrarily close to 1 upon choosing a suitable t, then a and b must be strongly cospectral. We intend now to provide a good bound for the threshold.

Assume now that

$$\sum_{r=0}^{d} \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}} = \delta.$$

Let $x = \left(\sqrt{(E_r)_{a,a}}\right)_{r=0,\dots,d}$ and $y = \left(\sqrt{(E_r)_{b,b}}\right)_{r=0,\dots,d}$. Note that these are unit vectors, and $\langle x, y\rangle = \delta$. Whence,

$$\langle x - y, x - y\rangle = 2 - 2\langle x, y\rangle = 2 - 2\delta.$$

As each entry of $\langle x - y, x - y\rangle$ is a square, it follows that, for all r,

$$\left(\sqrt{(E_r)_{a,a}} - \sqrt{(E_r)_{b,b}}\right)^2 \leq 2 - 2\delta,$$

and since, $(E_r)_{a,a} \leq 1$ and $(E_r)_{b,b} \leq 1$, we finally have our upper bound:

$$((E_r)_{a,a} - (E_r)_{b,b})^2 \leq 2(2 - 2\delta). \tag{7.2.1}$$

We next derive a lower bound on $|(E_r)_{a,a} - (E_r)_{b,b}|$. We are assuming A has exactly $(d+1)$ distinct eigenvalues and $n = |V(X)|$. Let N_a and N_b respectively denote the $n \times (d+1)$ matrices with columns consisting of the vectors $E_r e_a$ and $E_r e_b$. Let F be the $(d+1) \times n$ matrix with $F_{r\ell} = \theta_r^{\ell-1}$. If W_a and W_b are the walk matrices of a and b respectively, then

$$W_a = N_a F, \quad W_b = N_b F$$

and

$$W_a^T W_a - W_b^T W_b = F^T(N_a^T N_a - N_b^T N_b)F. \tag{7.2.2}$$

The matrices $N_a^T N_a$ and $N_b^T N_b$ are diagonal with

$$(N_a^T N_a)_{r,r} = (E_r)_{a,a}, \quad (N_b^T N_b)_{r,r} = (E_r)_{b,b}.$$

Hence

$$F^T(N_a^T N_a - N_b^T N_b)F = \sum_{r=0}^{d}((E_r)_{a,a} - (E_r)_{b,b})F^T e_r e_r^T F. \tag{7.2.3}$$

Let η denote the maximum value of $|(E_r)_{a,a} - (E_r)_{b,b}|$. Then by the triangle inequality

$$\left\| \sum_r ((E_r)_{a,a} - (E_r)_{b,b}) F^T e_r e_r^T F \right\| \le \eta \sum_r \left\| F^T e_r e_r^T F \right\|, \tag{7.2.4}$$

where we are using the trace-norm. We have

$$\left\| F^T e_r e_r^T F \right\|^2 = \operatorname{tr}(F^T e_r e_r^T F\, F^T e_r e_r^T F) = (e_r^T F F^T e_r)^2,$$

whence $\|F^T e_r e_r^T F\| = (FF^T)_{r,r}$ and therefore the right side in (7.2.4) is equal to $\eta \operatorname{tr}(FF^T)$.

If a and b are not cospectral then, from Theorem 6.2.1, $W_a^T W_a \ne W_b^T W_b$ and, since these matrices are integer matrices, the norm of $W_a^T W_a - W_b^T W_b$ is at least 1. So Equations (7.2.2), (7.2.3) and (7.2.4) imply that

$$\frac{1}{\operatorname{tr}(FF^T)} \le \eta.$$

Combining this with Equation (7.2.1) yields that

$$\frac{1}{\operatorname{tr}(FF^T)} \le \max_r |(E_r)_{a,a} - (E_r)_{b,b}| \le 2\sqrt{1-\delta},$$

and so we have proved that if a and b are not cospectral, then

$$\delta \le 1 - \frac{1}{4 \operatorname{tr}(FF^T)^2}$$

Denote the largest eigenvalue by ρ. Since

$$\operatorname{tr}(FF^T) = \sum_{r=0}^{d} \sum_{i=0}^{n-1} \theta_r^{2i} \le (d+1) \sum_{i=0}^{n-1} \rho^{2i} = (d+1) \frac{\rho^{2n}-1}{\rho^2-1} \le n\rho^{2n}.$$

Therefore

$$\delta \le 1 - \frac{1}{4n^2 \rho^{4n}}.$$

The result now follows from $\|D_a(t) - D_b\|^2 = 2 - 2|U(t)_{a,b}|^2$, and from $|U(t)_{a,b}|^2 \le \delta^2$, which is a consequence of Equations (7.1.1) and (7.1.2). □

7.3 Ratio Condition

In Corollary 1.4.2 we saw that if perfect state transfer happens between a and b, then both these vertices are periodic at double the time. In the language of density matrices, vertex a is periodic at time t if and only if $D_a(t) = D_a$, that is,

$$\left(\sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} E_r\right) D_a \left(\sum_{r=0}^{d} \mathrm{e}^{-\mathrm{i}t\theta_r} E_r\right) = D_a,$$

and equivalently,

$$\sum_{r,s=0}^{d} \mathrm{e}^{\mathrm{i}t(\theta_r-\theta_s)} E_r D_a E_s = \sum_{r,s=0}^{d} E_r D_a E_s.$$

The matrices $\{E_r D_a E_s\}_{r,s}$ are orthogonal, thus the equality above is equivalent to having, for all r and s so that $E_r D_a E_s \neq 0$, that is, for all θ_r and θ_s in the eigenvalue support of a,

$$\mathrm{e}^{\mathrm{i}t(\theta_r-\theta_s)} = 1.$$

This can also be obtained immediately as a consequence of Lemma 7.1.1 by making $a = b$, and noting that $\mathrm{e}^{\mathrm{i}t\theta_r}$ will be constant for all r whenever $E_r e_a \neq 0$.

The *ratio condition* on the eigenvalue support of a vertex a holds if, for any four eigenvalues θ_r, θ_s, θ_k, θ_ℓ in the eigenvalue support of a with $\theta_k \neq \theta_\ell$, we have

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}.$$

7.3.1 Corollary. *A graph X is periodic at the vertex a if and only if the ratio condition holds at a.*

Proof. Periodicity at a is equivalent to having, for all θ_r and θ_s in its eigenvalue support,

$$\mathrm{e}^{\mathrm{i}t(\theta_r-\theta_s)} = 1.$$

Hence there are integers $m_{r,s}$ such that

$$t(\theta_r - \theta_s) = 2m_{r,s}\pi$$

and consequently

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} = \frac{m_{r,s}}{m_{k,\ell}} \in \mathbb{Q}.$$

Hence if X is periodic at a, the ratio condition holds.

Conversely, if the ratio condition holds, then taking θ_k and θ_ℓ distinct and in the eigenvalue support, it follows that

$$\frac{m_{k,\ell}}{\theta_k - \theta_\ell}(\theta_r - \theta_s) \in \mathbb{Z}$$

for all r and s, and therefore X is periodic at a at time $t = 2m_{k,\ell}\pi/(\theta_k - \theta_\ell)$. □

7.4 Algebraic Numbers

For the next section, some knowledge in algebraic number theory is desirable. Now we will recall a few concepts and results.

A complex number is an *algebraic number* if it is the root of a polynomial with integer coefficients. It is an *algebraic integer* if it is the root of a monic polynomial with integer coefficients.

7.4.1 Lemma. *A complex number μ is an algebraic integer if and only if it is the eigenvalue of a matrix with integer coefficients.*

Proof. One direction follows because the characteristic polynomial of a matrix with integer coefficients is a monic polynomial with integer coefficients. The other is consequence of the fact that the polynomial $p(x) = x^n + a_{n-1}x^{n-1} + ... + a_0$ is the characteristic polynomial of the matrix

$$\begin{pmatrix} 0 & 0 & 0 & \dots & 0 & -a_0 \\ 1 & 0 & 0 & \dots & 0 & -a_1 \\ 0 & 1 & 0 & \dots & 0 & -a_2 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & -a_{n-2} \\ 0 & \dots & 0 & 0 & 1 & -a_{n-1} \end{pmatrix}$$

□

The matrix that appears in the proof above is called the *companion matrix* of the polynomial $p(x)$. It is well-known that the eigenvalues of the companion matrix are the roots of $p(x)$, and that it is diagonalized by the inverse of the Vandermonde matrix whose rows correspond to the roots of $p(x)$.

If μ is eigenvalue of M and ν is eigenvalue of N, then $\mu+\nu$ is eigenvalue of $M \otimes I + I \otimes N$, and $\mu\nu$ is eigenvalue of $M \otimes N$. As a consequence of the lemma, we have the corollary.

7.4.2 Corollary. *The set of algebraic integers is closed under addition and multiplication.* □

It is not difficult to show that the same conclusion holds for algebraic numbers.

For the algebraic integers, a stronger statement also follows.

7.4.3 Theorem. *Roots of monic polynomials whose coefficients are algebraic integers are algebraic integers themselves.* □

The minimal polynomial of an algebraic number μ is the monic polynomial $p(x) \in \mathbb{Q}[x]$ of minimal degree such that $p(\mu) = 0$. It is a useful exercise to use the Euclidean Algorithm to show that the minimal polynomial of an algebraic integer has integer coefficients, and also to show that the minimal polynomial of an algebraic number is irreducible in $\mathbb{Q}[x]$. The *algebraic conjugates* of an algebraic number μ are the other roots of its minimal polynomial.

For every algebraic number μ, there is another (unique!) algebraic number ν so that $\mu\nu = 1$. In fact, if $p(x) = \sum_{j=0}^{n} a_j x^j$ is the minimal polynomial of μ, and because $p(x)$ is irreducible, it must be that $a_0 \neq 0$, and then $\nu = -a_0^{-1}(\sum_{j=1}^{n} a_j x^j)$. This is the key step in showing that the set of algebraic numbers forms a field. We are interested in the intermediate fields that lie between $\mathbb{Q}$ and the algebraic numbers.

Let $\mathbb{Q}[x]$ denote the ring of all finite sums of monomials on the element $\{x\}$ with rational coefficients. If some monomial can be written as a linear combination of smaller powers with rational coefficients, then x is an algebraic number. Otherwise, we can think of x as an indeterminate (or variable), and $\mathbb{Q}[x]$ as the ring of polynomials on x. We use $\mathbb{Q}[x_1, ..., x_n]$ to denote the ring of all finite sums of monomials on the elements $\{x_1, ..., x_n\}$ with coefficients from $\mathbb{Q}$.

If μ is an algebraic number with minimal polynomial $p(x)$, and if $\langle p(x)\rangle = \{q(x)p(x) : q(x) \in \mathbb{Q}[x]\}$ denotes the *ideal* generated by $p(x)$ in $\mathbb{Q}[x]$, the First Isomorphism Theorem says that

$$\mathbb{Q}[\mu] \cong \mathbb{Q}[x]/\langle p(x)\rangle. \tag{7.4.1}$$

Thus, any other algebraic number ν whose minimal polynomial is also $p(x)$ generates the extension $\mathbb{Q}[\nu]$ isomorphic to $\mathbb{Q}[\mu]$. As $\mathbb{Q}$ is a field, $\mathbb{Q}[x]$ is a principal ideal domain and thus the ideal generated by irreducible elements is maximal. The quotient of a ring by a maximal ideal is a field, and therefore $\mathbb{Q}[\mu]$ is a field. Alternatively, we can easily show that if $p(x)$ is the minimal polynomial of μ and $q(\mu) \in \mathbb{Q}[\mu]$ is non-zero, then the inverse of $q(\mu)$ can be obtained applying the extended Euclidean algorithm, because $p(x)$ is irreducible and does not divide $q(x)$, therefore there are polynomials $a(x)$ and $b(x)$ so that

$$a(x)p(x) + b(x)q(x) = 1,$$

hence $b(\mu)q(\mu) = 1$.

If $p(x) \in \mathbb{Q}[x]$ and $\{\mu_1, ..., \mu_n\}$ are its roots, then $\mathbb{Q}[\mu_1, ..., \mu_n]$ is a field extension of $\mathbb{Q}$ that contains all roots of $p(x)$, and in fact, it is minimal with this property. It is called the *splitting field* of $p(x)$ over $\mathbb{Q}$.

Any bijection σ from a field $\mathbb{F}$ to itself that preserves the field structure is called a field automorphism. This means that $(\mu+\nu)^\sigma = (\mu)^\sigma + (\nu)^\sigma$, and $(\mu\nu)^\sigma = (\mu)^\sigma(\nu)^\sigma$, for all $\mu, \nu \in \mathbb{F}$. Assume $\mathbb{F}$ is a field that contains $\mathbb{Q}$. Note that $0^\sigma = 0$, and $1^\sigma = 1$, for all field automorphisms, and it is not difficult to extend these observations and show that $\mu^\sigma = \mu$ for all $\mu \in \mathbb{Q}$. Moreover, if μ is an algebraic number with minimal polynomial $p(x) = \sum a_j x^j$, then

$$0 = 0^\sigma = (p(\mu))^\sigma = p^\sigma(\mu^\sigma) = \sum_j a_j \mu^\sigma,$$

thus μ^σ is also a root of $p(x)$. Using the inverse of σ, it is immediate to show that $p(x)$ is in fact the minimal polynomial of μ.

If $\mathbb{Q}[\mu_1, ..., \mu_n]$ is an algebraic extension of $\mathbb{Q}$, and if $\mu \in \mathbb{Q}[\mu_1, ..., \mu_n]$, Galois showed that μ is fixed by all automorphisms of $\mathbb{Q}[\mu_1, ..., \mu_n]$ if and only if $\mu \in \mathbb{Q}$.

As we saw, a consequence of Equation (7.4.1) is that if μ and μ' are roots of the same minimal polynomial $p(x)$, then $\mathbb{Q}[\mu] \cong \mathbb{Q}[\mu']$, and the field isomorphism that takes one to the other can be extended to a field automorphism of the splitting field of $p(x)$. If M is an integer matrix, and μ is one of its eigenvalues with correspondent projector E_μ, then the entries of this matrix lie in $\mathbb{Q}[\mu]$, and $\mu' = \mu^\sigma$ is also an eigenvalue of M, with corresponding projector E_μ^σ (obtained from E_μ upon applying σ entry-wise).

An algebraic integer μ whose minimal polynomial has degree two is called a *quadratic integer*. A real number μ is a quadratic integer if and only if there are integers a, b and Δ such that Δ is square-free and one of the following cases holds.

(i) $\mu = a + b\sqrt{\Delta}$ and $\Delta \equiv 2, 3 \pmod 4$.

(ii) $\mu = \frac{1}{2}\left(a + b\sqrt{\Delta}\right)$, $\Delta \equiv 1 \pmod 4$, and either a and b are both even or both odd.

7.5 Perron-Frobenius Theory

Let M be a real $n \times n$ matrix with nonnegative entries. For example, the adjacency matrix of a graph. This matrix is called primitive if, for some integer k, $M^k > 0$, and it is called irreducible if for all indices i and j, there is an integer k so that $(M^k)_{ij} > 0$. All primitive matrices are irreducible, but the converse is not necessarily true.

It is not difficult to see that the adjacency matrix of a graph is irreducible if and only if the graph is connected, and also that the adjacency matrix of a connected bipartite graph is irreducible but not primitive.

Results below are part of what is usually known as the Perron-Frobenius theory. This theory applies generally to matrices which are assumed to be irreducible and nothing else. We shall however add the hypothesis that the matrices are also symmetric, as the proofs become simpler and will be enough for our purposes.

7.5.1 Lemma. *Let M be a nonnegative symmetric matrix, $M \neq 0$. If λ is the largest eigenvalue of M, then $\lambda > 0$.*

Proof. Follows immediately from $\operatorname{tr} M \geq 0$. □

For any vector $u \in \mathbb{R}^n$, and symmetric matrix M, define

$$R_M(u) = \frac{u^T M u}{u^T u}.$$

This is known as the Rayleigh quotient of u with respect to M. Note that $R_M(\alpha u) = R_M(u)$ for all $\alpha \neq 0$, so we shall typically assume $u \neq 0$ has been normalized. In a sense, this is a measurement of how much M displaces u, also proportional to how much M stretches or shrinks u. Therefore one should expect that this is maximum when u is an eigenvector of M, corresponding to a large eigenvalue.

7.5.2 Lemma. *If u is eigenvector of M with eigenvalue θ, then $R_M(u) = \theta$. If λ is the largest eigenvalue of M, then, for all $v \in \mathbb{R}^n$, $R_M(v) \leq \lambda$. Equality holds for some v only if v is eigenvector for λ.*

Proof. The first claim is straightforward. Let now $M = \sum_{r=0}^{d} \theta_r E_r$ be the spectral decomposition of M. Assume λ_0 is the largest eigenvalue, and that v is a normalized vector. Then

$$\begin{aligned} R_M(v) = v^T M v &= \theta_0(v^T E_0 v) + \theta_1(v^T E_1 v) + ... + \theta_d(v^T E_d v) \\ &\leq \theta_0((v^T E_0 v) + (v^T E_1 v) + ... + (v^T E_d v) = \theta_0. \end{aligned}$$

Equality holds if and only if $(v^T E_r v) = 0$ for all $r > 0$, which is the same as saying that v belongs to the θ_0-eigenspace. □

7.5.3 Lemma. *Let M be symmetric, non-negative and irreducible, with largest eigenvalue λ. There is a corresponding eigenvector u to λ so that $u > 0$.*

Proof. Let v be a normalized eigenvector for λ, and define u to be made from v by taking the absolute value at each entry (also denoted by $u = |v|$). Note that u is still normalized, and, moreover

$$\lambda = R_M(v) = |R_M(v)| \leq R_M(u) \leq \lambda.$$

(Second equality follows from $\lambda > 0$. First inequality is simply the triangle inequality. Second follows from Lemma 7.5.2.)

Hence $R_M(u) = \lambda$, and u is an eigenvector for λ, with $u \geq 0$. To see that $u > 0$, note that as M is irreducible, it follows easily that $I + M$ is primitive, and so there is a k so that $(I + M)^k > 0$. The vector u is also eigenvector for this matrix (with eigenvalue $(1 + \lambda)^k$), but

$$0 < (I + M)^k u = (1 + \lambda)^k u,$$

implying $u > 0$. □

7.5.4 Lemma. *The largest eigenvalue λ of a symmetric, non-negative and irreducible matrix is simple.*

Proof. From the proof of the past lemma, we know that no eigenvector for λ contains an entry equal to 0. No subspace of dimension larger than 1 can be such that all of its non-zero vectors have no non-zero entries. □

And finally:

7.5.5 Lemma. *Let M be symmetric, non-negative and irreducible. Let λ be its largest eigenvalue. Let μ be any other eigenvalue. Then $\lambda \geq |\mu|$, and, moreover, if $-\lambda$ is an eigenvalue, then M^2 is not irreducible.*

Proof. Let v be an eigenvector for μ. As v is orthogonal to the positive eigenvector corresponding to λ, at least one entry of v is negative. Thus

$$|\mu| = |R_M(v)| < R_M(|v|) \leq \lambda.$$

Now note that λ^2 is the largest eigenvalue of M^2 (which is, still, symmetric and non-negative). If $-\lambda$ is eigenvalue of M, then the eigenspace of λ^2 in M^2 is at least 2-dimensional, thus M^2 cannot be irreducible. □

It is quite surprising at first sight that the hypothesis on M being symmetric can be dropped entirely from the results above. The geometric intuition remains the same: a nonnegative irreducible matrix acts in the nonnegative orthant and there it encounters a unique direction which is an eigenvector. In the notes we leave some references for these more general results.

7.6 Periodicity and Integrality

We saw in Corollary 7.3.1 that periodicity is equivalent to a condition on the ratio of differences of eigenvalues. This condition implies a severe restriction on the algebraic nature of the eigenvalues that lie in the eigenvalue support of a periodic vertex, as we will see below.

In this section, we will assume the results in Section 7.4.

7.6.1 Theorem. *Assume $S = \{\theta_0, ..., \theta_d\}$ is a set of real algebraic integers, closed under taking algebraic conjugates, and with $d \geq 3$. Then, for all*

r, s, k, ℓ with $\theta_k \neq \theta_\ell$, we have

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}$$

if and only if either of the following holds.

(a) The elements in S are integers.

(b) The elements in S are quadratic integers, and, moreover, there is a square-free integer $\Delta > 1$, an integer a and integers $b_0, ..., b_d$ so that $\theta_r = \frac{1}{2}(a + b_r\sqrt{\Delta})$.

Proof. It is straightforward to verify that if either of our stated conditions holds, then the stated ratio condition is satisfied.

We assume the ratio condition holds. If two elements in S are integers, say θ_0 and θ_1 then since the ratio condition asserts that

$$\frac{\theta_r - \theta_0}{\theta_1 - \theta_0} \in \mathbb{Q},$$

we conclude that all elements of S are integers.

So we may assume at most one element of S is an integer. Let θ_0 and θ_1 be two distinct elements of S; we will show that $(\theta_1 - \theta_0)^2$ is an integer. By the ratio condition, if $\theta_r, \theta_s \in S$ there is a rational number $a_{r,s}$ such that

$$\theta_r - \theta_s = a_{r,s}(\theta_1 - \theta_0)$$

and therefore

$$\prod_{r \neq s}(\theta_r - \theta_s) = (\theta_1 - \theta_0)^{d^2-d} \prod_{i \neq j} a_{r,s}.$$

The product on the left is fixed by any field automorphism of $\mathbb{Q}[\theta_0, ..., \theta_d]$, thus it is an integer, and the product of the $a_{r,s}$'s is rational, and hence

$$(\theta_1 - \theta_0)^{d^2-d} \in \mathbb{Q}.$$

Since $\theta_1 - \theta_0$ is an algebraic integer, this implies that

$$(\theta_1 - \theta_0)^{d^2-d} \in \mathbb{Z}.$$

Suppose m is the least positive integer such that $(\theta_1 - \theta_0)^m$ is an integer. Then there are m distinct conjugates of $\theta_1 - \theta_0$ of the form

$$\beta e^{2\pi i k/m} \qquad (k = 0, \dots, m-1)$$

where β is the positive real m-th root of an integer. Since the elements of S are real and closed under taking conjugates, we conclude that $m \leq 2$.

Therefore $\theta_1 - \theta_0$ is either an integer or an integer multiple of the square root of a square-free integer Δ (we assume $\theta_1 - \theta_0$ is a multiple of $\sqrt{\Delta}$ in both cases for convenience, and take $\Delta = 1$ in the former case). Since

$$(\theta_r - \theta_s)^2 = a_{r,s}^2(\theta_1 - \theta_0)^2$$

it follows that $(\theta_r - \theta_s)^2$ is rational and therefore it is an integer. So $\theta_r - \theta_s$, again, is multiple of the square root of an integer $\Delta_{r,s}$. More so, its square free part is the same as the one $(\theta_1 - \theta_0)^2$, thus $\Delta_{r,s} = \Delta$, for all r and s.

Therefore there are integers m_r such that, for each r,

$$\theta_r = \theta_0 - m_r\sqrt{\Delta}. \tag{7.6.1}$$

If we sum this over the elements of S we find that

$$|S|\theta_0 - \sqrt{\Delta}\sum_r m_r = \sum_r \theta_r \in \mathbb{Z},$$

the last claim following from the fact that the sum is fixed by all automorphisms of the extension containing the elements of S. Therefore θ_0 lies in $\mathbb{Q}(\sqrt{\Delta})$, and so do all other elements of S. The fact that their rational parts are the same follows immediately from Equation (7.6.1). □

The results in Section 7.5 imply that if θ_0 is the largest eigenvalue of a connected graph, then it belongs to the eigenvalue support of all vertices.

7.6.2 Corollary. *Suppose X is an integer weighted connected graph with at least two vertices and let S be the eigenvalue support of the vertex a. Then X is periodic at a if and only if either of the following holds.*

(a) The eigenvalues in S are integers.

(b) The elements in S are quadratic integers, and, moreover, there is a square-free integer $\Delta > 1$, an integer a and integers $b_0, ..., b_d$ so that $\theta_r = \frac{1}{2}(a + b_r\sqrt{\Delta})$.

Moreover, if the either condition holds, and taking $\Delta = 1$ if the eigenvalues are all integers, let

$$g = \gcd\left\{\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}\right\}_{\theta_r \in S}.$$

Then the smallest positive τ so that $D_a(\tau) = D_a$ is $\tau = \frac{2\pi}{g\sqrt{\Delta}}$, and if $D_a(t) = D_a$, then t is an integer multiple of t.

Proof. As X is connected with at least two vertices, $|S| \geq 2$. If θ_r and θ_s are algebraic conjugates, then E_r and E_s are algebraic conjugates and so $E_r e_a = 0$ if and only if $E_s e_a = 0$. Therefore S contains all algebraic conjugates of each of its elements. If $|S| = 2$, then either both elements of S are integers, or they are roots of a quadratic polynomial (and (b) holds). So we can assume that $|S| \geq 3$, and therefore apply Corollary 7.3.1 and Theorem 7.6.1.

If periodicity occurs at time t, we can write

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

where τ is a suitable real number. From the proof of Corollary 7.3.1, we see that

$$\tau \frac{\theta_0 - \theta_s}{g\sqrt{\Delta}} \in \mathbb{Z},$$

so, from the choice of g, it follows that τ is an integer. □

7.7 Consequences of Integrality

One of the most important consequences of Corollary 7.6.2 is that the distinct eigenvalues in the support of a periodic vertex differ by at least 1. This is not the standard behaviour for typical vertices in graphs, as the two results below will indicate.

The first is an attempt to formally justify why is it so difficult to find examples of periodic vertices or perfect state transfer (as the latter phenomenon implies the former). Among such examples, it is even rarer that the graph looks sparse—the second result will explain why is this the case.

Recall that the dual degree of a vertex is the size of its eigenvalue support minus 1. Lemma 5.2.5 stated that if a is a vertex of $V(X)$ with covering radius r and dual degree s^*, then $r \leq s^*$.

7.7.1 Corollary. *There are only finitely many connected graphs with maximum valency at most k which contain a periodic vertex.*

Proof. Suppose X is a connected graph where vertex a is periodic, and let S be its eigenvalue support. From Corollary 7.6.2, the distance between two distinct elements of S is at least 1, and since all eigenvalues of X lie in the interval $[-k, k]$, we see that $|S| \leq 2k+1$. In other terms we have shown that the dual degree of a is at most $2k$ and so, by Lemma 5.2.5, it follows that the covering radius of a is at most $2k$. Since the maximum valency is bounded, it follows that $|V(X)|$ is bounded. □

Following, let us now explore another consequence of the fact that the covering radius of a is at most the dual degree.

7.7.2 Corollary. *Assume X has m edges. If a is a periodic vertex with covering radius r, then*

$$r^3 \leq 54m.$$

Proof. We list the eigenvalues of A with possible repetition by $\lambda_1, \ldots, \lambda_n$, assuming that $\lambda_1^2 \geq \ldots \geq \lambda_n^2$. The trace of $A(X)^2$ is the sum of the degrees, and also the sum of the eigenvalues squared, when counted with multiplicity. Thus,

$$\lambda_j^2 \leq \frac{2m}{j}.$$

Let S be the eigenvalue support of a. With a periodic, the eigenvalues in S are separated by at least 1, thus, for all $1 \leq j \leq n$,

$$(|S| - j + 1) \leq 2|\lambda_j| + 1.$$

Thus,

$$r + 1 \leq |S| \leq 2\sqrt{\frac{2m}{j}} + j.$$

Make $j = \lceil \sqrt[3]{2m} \rceil$. Note that $j \leq n$, and thus

$$r \leq 3\sqrt[3]{2m}.$$ □

As we have already seen, if there is perfect state transfer between a and b, then both are periodic. Hence, both results above can be seen as consequences of Corollary 7.6.2 to limit when is perfect state transfer possible in a graph. In the next section, we will see that we can also use this corollary provide a characterization.

7.8 Perfect state transfer

The three inequalities (7.1.1), (7.1.2) and (7.1.3) and their respective equality characterizations in the subsequent lemmas allow for a characterization of perfect state transfer between a and b. They must be parallel and cospectral, hence strongly cospectral, and the $e^{it\theta_r}$ must alternate sign according to $(E_r)_{a,b}$. With a and b both periodic, we can use Corollary 7.6.2 to ask when eigenvalues which are integers or quadratic integers of the prescribed form give the correct alternating pattern. In the following theorem, we make this analysis explicit.

Given a rational m and a prime p, we can write $m = p^\alpha \frac{r}{s}$, where r and s are integers not divisible by p. Then the *p-adic norm* of m is defined by

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

Thus, if m is integer, the larger the power of p dividing m is, the smaller its p-adic norm is.

7.8.1 Theorem. *Let a and b be vertices in a graph X, and assume the eigenvalue support of a consists of eigenvalues $S = \{\theta_0, \ldots, \theta_k\}$. There is perfect state transfer between a and b if and only if:*

(a) Vertices a and b are strongly cospectral;

(b) The eigenvalues in S are either integers or quadratic integers, and, moreover, there are integers $a, \Delta, b_0, \ldots, b_k$, with Δ positive and square-free, so that

$$b_r = \frac{1}{2}(a + b_r\sqrt{\Delta});$$

(c) There is a non-negative integer α so that

- *$(E_r)_{a,b} > 0$ if and only if $|(\theta_0 - \theta_r)/\sqrt{\Delta}|_2 < 2^{-\alpha}$,*
- *$(E_r)_{a,b} < 0$ if and only if $|(\theta_0 - \theta_r)/\sqrt{\Delta}|_2 = 2^{-\alpha}$.*

If the above conditions hold, let

$$g = \gcd\left\{\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}\right\}_{r=0,\ldots,k}.$$

Then the minimum time we have perfect state transfer between a and b is $\tau = \pi/g\sqrt{\Delta}$, and any other time it occurs is an odd multiple of τ.

Proof. We have seen that conditions (a) and (b) are necessary, so we assume they hold and prove that perfect state transfer is equivalent to condition (c). Note first that (a) implies the eigenvalue support of a and b are the same. Let $\tau = t\frac{\pi}{g\sqrt{\Delta}}$. We have

$$U(\tau)e_a = \lambda e_b$$

if and only if, for all θ_r, $\mathrm{e}^{\mathrm{i}\tau\theta_r} E_r e_a = \lambda E_r e_b$. We can assume θ_0 is the spectral radius, and thus E_0 is a non-negative matrix. Thus the condition is equivalent to having $\lambda = \mathrm{e}^{\mathrm{i}\tau\theta_0}$, and

$$\mathrm{e}^{\mathrm{i}\tau(\theta_0-\theta_r)} = \pm 1,$$

where the sign is determined by whether $E_r e_a = \pm E_r e_b$, or equivalently the sign of $(E_r)_{a,b}$. If $m_1, \cdots, m_k$ are reals satisfying

$$t\frac{\pi}{g\sqrt{\Delta}}(\theta_0 - \theta_r) = m_r\pi,$$

perfect state transfer is equivalent to m_r being an even integer if $(E_r)_{a,b} > 0$, and m_r being an odd integer if $(E_r)_{a,b} < 0$. As t is constant, it must be an odd positive integer that plays no role whether it happens or not. Thus, perfect state transfer is equivalent to $(\theta_0 - \theta_r)/g\sqrt{\Delta}$ being even if $(E_r)_{a,b} > 0$, and $(\theta_0 - \theta_r)/g\sqrt{\Delta}$ being odd if $(E_r)_{a,b} < 0$. This is precisely equivalent to the condition stated in (c). □

Note that the minimum time perfect state transfer occurs depends only on the eigenvalue support of the vertex a. The following corollary is an immediate consequence.

7.8.2 Corollary. *In the graph X, if there is perfect state transfer between a and b, and between a and c, then $a = c$.* □

The conditions presented in the Theorem are quite useful, in the sense that they allow for an efficient and effective method of testing whether perfect state transfer occurs, given the graph X. Efficient here meaning precisely "in a time bounded by a polynomial in $n = |V(X)|$", and effective meaning "in exact arithmetic".

In Theorem 6.8.2, the characterization of strongly cospectral vertices in terms of whether $\phi(X\backslash a, t) = \phi(X\backslash b, t)$ and the poles of $\phi(X\backslash ab, t)/\phi(X, t)$

are simple can be tested in polynomial time in n. The multiplicity of θ as a pole of $\phi(X\backslash a,t)/\phi(X,t)$ indicates whether it lies in the eigenvalue support of a or not, as a consequence of Corollary 4.5.2. This multiplicity is equal to one if and only if θ is a root of the integral polynomial

$$\frac{\phi(X,t)}{\gcd\{\phi(X,t),\phi(X\setminus a,t)\}}.$$

Thus, we can test with symbolic arithmetic whether the eigenvalues in the support of a are integers or quadratic integers. As the candidates lie within a given interval of size bounded by a polynomial in n, this can also be carried out efficiently.

Once the eigenvalues have been found, if they satisfy condition (b) of Theorem 7.8.1, then it is easy to check condition (c).

7.9 Bipartite and Regular Graphs

We spell out yet more consequences of Theorem 7.6.1.

7.9.1 Lemma. *If X is bipartite and a is a periodic vertex, then either the eigenvalues in the eigenvalue support of a are all integers, or else they are integer multiples of $\sqrt{\Delta}$ for some square-free integer Δ.*

Proof. Suppose X is bipartite and the eigenvalue support S of the vertex a contains a non-integer eigenvalue. Then each element of S can be written in the form

$$\frac{1}{2}(a+b_r\sqrt{\Delta})$$

for some r, where a and b_r are integers and Δ is a square-free integer, but by Lemma 5.2.4 the set S is closed under multiplication by -1, and therefore $a=0$. Since eigenvalues are algebraic integers, it follows that b_r is even. □

We derive an interesting consequence of the previous result.

7.9.2 Lemma. *If X is connected, bipartite and $\det(A)=\pm1$, and perfect state transfer occurs on X, then $X=P_2$.*

Proof. If X is periodic at the vertex a, then the eigenvalue support of a consists of integers, or of integer multiples of $\sqrt{\Delta}$ for a square-free integer Δ. Since $\det(A)=\pm1$, the product of the eigenvalues distinct from θ is equal to θ^{-1}. Therefore θ^{-1} is an algebraic integer, and this implies that $\theta = \pm 1$. It is straightforward to show that in this case the connected component of X that contains a is P_2. □

The largest eigenvalue of a regular graph is the degree of the vertices, ergo an integer. In this case, we can also restrict even further the candidates to lie in the eigenvalue support of a periodic vertex.

7.9.3 Lemma. *Suppose X is connected and its spectral radius is an integer. Then if X is periodic at a, all elements of the eigenvalue support of a are integers.*

Proof. Assume by way of contradiction that X is periodic at a and some element θ of S is not an integer. Then the algebraic conjugate $\bar{\theta}$ of θ lies in S as does the spectral radius ρ of X. By the ratio condition

$$\frac{\theta - \rho}{\bar{\theta} - \rho} \in \mathbb{Q}$$

and therefore, since $\bar{\rho} = \rho$,

$$\frac{\theta - \rho}{\bar{\theta} - \rho} = \frac{\bar{\theta} - \rho}{\theta - \rho}.$$

Hence

$$(\theta - \rho)^2 = (\bar{\theta} - \rho)^2,$$

from which we deduce that

$$\theta + \bar{\theta} = 2\rho.$$

Since no eigenvalue if X is greater than ρ we infer that $\theta = \rho$, which contradicts our assumption on θ. □

The main application of the above lemma is to regular graphs.

7.10 No Control

We will prove that a controllable vertex cannot be periodic, and thus cannot be involved in perfect state transfer. This will be yet another application of Corollary 7.6.2. For this we need the following:

7.10.1 Lemma. *Let X be a graph with $n = |V(X)|$. If σ is the minimum distance between two eigenvalues of X, then*

$$\sigma^2 < \frac{12}{n+1}.$$

Proof. Assume that the eigenvalues of X in non-increasing order are $\theta_1, \ldots, \theta_n$. If we have

$$M := A \otimes I - I \otimes A,$$

then the eigenvalues of M are the numbers

$$\theta_i - \theta_j, \quad 1 \le i, j \le n.$$

Now

$$M^2 = A^2 \otimes I + I \otimes A^2 - 2A \otimes A,$$

and consequently, if $m = |E(X)|$, then

$$\sum_{i,j=1}^{n} (\theta_i - \theta_j)^2 = \operatorname{tr}(M^2) = 2n \operatorname{tr}(A^2) = 4nm.$$

Since

$$\theta_i - \theta_j \ge (i - j)\sigma,$$

we have

$$\sum_{i,j=1}^{n} (\theta_i - \theta_j)^2 \ge \sigma^2 \sum_{i,j=1}^{n} (i - j)^2.$$

As

$$\sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6},$$

we find that

$$\sum_{i,j=1}^{n} (i-j)^2 = 2n \sum_{i=1}^{n} i^2 - 2 \left(\sum_{i=1}^{n} i \right)^2 = \frac{n^2(n^2-1)}{6},$$

and since $m \le n(n-1)/2$, this yields

$$\sigma^2 \frac{n^2(n^2-1)}{6} \le 4nm \le 2n^2(n-1).$$

This gives our stated bound but with $\le$ in place of $<$. To achieve strictness we note that if equality were to hold then $m = n(n-1)/2$ and $X = K_n$. Since $\sigma(K_n) = 0$, we are done. □

7.10.2 Theorem. *Let X be a connected graph on at least four vertices. If we have a periodic vertex a in X, then a is not controllable.*

Proof. Let $n = |V(X)|$. We assume by way of contradiction that (X, a) is controllable. Then the eigenvalue support of a contains all eigenvalues of X and these eigenvalues are distinct. From Corollary 7.6.2 we know that the separation $\sigma(X)$ between distinct eigenvalues is at least 1.

By Lemma 7.10.1 we can assume that $n = |V(X)| \leq 10$. This leaves us with six cases. First suppose $\Delta = 1$. Assume $n = 10$. Then the sum of the squares of the eigenvalues of X is bounded below by the sum of the squares of the integers from -4 to 5, which is 85, and hence the average valency of a vertex is at least 8.5 (We are now going to use the well-known fact that the average valency of a graph is a lower bound to the largest eigenvalue.) This implies that $\theta_0 = 9$, not 5, consequently the sum of the squares of the eigenvalues is at least

$$85 - 25 + 81 = 141,$$

and now the average valency is 14.1, which is impossible. The cases where n is 7, 8 or 9 all yield contradictions in the same way. If $\Delta > 1$, it is even easier to derive contradictions.

Next, brute force computation (using Sage [54]) shows that the path P_4 is the only graph on 4, 5 or 6 vertices where the minimum separation between consecutive eigenvalues is at least 1. The positive eigenvalues of P_4 are

$$(\sqrt{5} \pm 1)/2,$$

so from Lemma 7.9.1 it cannot contain a periodic vertex. □

Note that the vertex a is controllable if and only if $\phi(X \setminus a, t)$ and $\phi(X, t)$ are coprime. By Lemma 5.3.4, if either of these polynomials is irreducible over $\mathbb{Q}$, the vertex a is controllable. It seems very plausible that almost graphs have irreducible characteristic polynomial, and therefore do not admit periodic vertices, and thus do not admit perfect state transfer as well.

Notes

Early versions of the ratio condition appear in Saxena et al [52] and in Christandl et al [20].

In Section 7.3 we condensed several results from algebraic number theory in a few paragraphs. Our favorite reference for those results is Cox [25]. Most of them date back at least to Galois. The characterization of quadratic integers is due to Dedekind.

Notes to pst is polytime paper, and qwalks and size of the graph papers. (It is Theorem 7.2 from Coutinho and Liu [24].)

Exercises

7-1. Prove (or research) each of the claims made on the paragraphs preceding Theorem 7.6.1.

7-2. Show that if a vertex is periodic according to the Laplacian matrix, then all eigenvalues in its eigenvalue support are integers.

7-3. Assume X has largest degree k. Find an upper bound for the largest eigenvalue of $L(X)$ in terms of k. Use it to conclude that there are only finitely many graphs with maximum degree k that contain a periodic vertex.

7-4. Prove a version of Theorem 7.6.1 where the elements satisfying the ratio condition are partitioned into two sets S_1 and S_2 of real algebraic integers, each with at least two elements and both closed under taking conjugates, and we can only assume that

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}$$

for when $\theta_r, \theta_s \in S_1$ and $\theta_k, \theta_\ell \in S_2$.

7-5. Let X be a graph on n vertices. Show that if X has simple eigenvalues and is periodic, then

$$n \leq 11.$$

Chapter 8

Recurrence and approximations

The concept of periodicity is key to the understanding and study of continuous-time quantum walks. Thus we have seen that if a graph X admits perfect state transfer from a to b at time t, then X is periodic at both vertices at time $2t$. In Section 2.7 we studied orbits of density matrices and proved (in Theorem 2.7.2) that quantum walks are "approximately" recurrent.

In this chapter we study recurrence and periodicity from a group theoretic perspective.

The main result we state and prove in this chapter in Kronecker's Theorem on Diophantine approximation.

8.1 The Unitary Group

The unitary group $U(d)$ is the group of $d \times d$ unitary matrices. It is a compact subset of $\mathbb{C}^{d^2}$. We have made extensive use of the fact that, if A is Hermitian, the matrices

$$\exp(\mathrm{i}tA), \qquad t \in \mathbb{R}$$

are unitary. They form a subgroup of the unitary group, subgroups of this form are so-called *1-parameter* subgroups. Each continuous quantum walk is a manifestation of a 1-parameter subgroup.

8.1.1 Lemma. *A matrix U is unitary if and only if there is a Hermitian matrix H such that $U = \exp(\mathrm{i}H)$.*

Proof. We have seen this condition is sufficient. For the necessity we note that is U is unitary it is normal and so has. a spectral decomposition

$$U = \sum_r \lambda_r E_r.$$

Since U is unitary, each eigenvalue λ_r has norm one and so we may assume

$$\lambda_r = \exp(\mathrm{i}\theta_r).$$

It follows that $U = \exp\Big(\sum_r \mathrm{i}\theta_r E_r\Big)$. □

The unitary group has a number of actions of interest to us. If $\|z\| = 1$ and Q is unitary, then $\|Qz\| = 1$. Hence $U(d)$ fixes the complex unit sphere. Its action on the unit sphere is transitive: if y and z are unit vectors, there is a unitary matrix Q such that $Qy = z$. If $U(t)$ is the transition matrix of a continuous walk with initial state z, then the set

$$\{U(t)z : t \in \mathbb{R}\}$$

is the orbit of z under the action of the 1-parameter subgroup given by $U(t)$.

For the second action, let Ω denote the set of positive semidefinite matrices of order $d \times d$. If $M \in \Omega$ and $Q \in U(d)$, then QMQ^* is positive semidefinite. This gives us an action of $U(d)$ on Ω. As $\mathrm{tr}(QMQ^*) = \mathrm{tr}(M)$, the density matrices of order $d \times d$ form a subset invariant under this action of $U(d)$. Since $\mathrm{rk}(QMQ^*) = \mathrm{rk}(M)$, we also see that $U(d)$ acts on the set of pure states.

The set of matrices $U(t)D)tU(-t)$ for $t \geq 0$ may be called the *forward orbit* of D_0. We have state transfer from D_0 to D_1 if and only if D_1 is in the forward orbit of D_0. In this case D_0 lies in the backwards orbit of D_0. If D_0 and D_1 are real, then D_1 lies in the backwards ordbit of D_0 if and only if it lies in the forwards orbit.

The set of positive definite matrices is also invariant under $U(d)$, this set is a Riemannian manifold (but this fact will play no explicit role in our work).

We restate some of the discussion from Section 2.7.

8.1.2 Lemma. *Let D_0 and D_1 be density matrices of order $d \times d$ and set $\mathcal{U} = \{U(t) : t \in \mathbb{R}\}$. Then:*

(a) *There is perfect state transfer from D_0 to D_1 under the continuous walk given by $U(t)$ if and only if D_1 lies in the forward orbit of D_0 under the action of $\mathcal{U}$.*

(b) *There is pretty good state transfer from D_0 to D_1 under the continuous walk given by $U(t)$ if and only if D_1 lies in the closure of the forward orbit of D_0 under the action of $\mathcal{U}$.* □

8.2 Discrete Subgroups

Formally, a subgroup H of a topological group G is a *discrete* if there is a cover of G by open sets, each of which contains exactly one element of H. For the groups of interest to us, we may say that H is discrete if no point in G is a limit point for H.

Thus the integers are a discrete subgroup of $\mathbb{R}$, but the subgroup H of $\mathbb{R}$ generated by $\{1, \sqrt{2}\}$ is discrete (every real number is limit point of H.)

A subgroup G of $\mathbb{R}^d$ is *discrete* if there is a positive real number ϵ such that the balls of radius ϵ about the elements of G are pairwise disjoint. A discrete subgroup of $\mathbb{R}$ consists of all integer multiples of some real number α. A subgroup of $\mathbb{R}$ is *dense* if its closure is $\mathbb{R}$.

8.2.1 Lemma. *An additive subgroup of $\mathbb{R}$ is either discrete or dense.* □

If $U(t)$ is the transition matrix for a continuous quantum walk, the map $t \mapsto U(t)$ is a homomorphism from $\mathbb{R}$ to the group

$$\mathcal{U} := \{U(t) : t \in \mathbb{R}\}.$$

8.2.2 Lemma. *If $U(t)$ is not contant, $\mathcal{U}$ is isomorphic to $\mathbb{R}$ or $\mathbb{R}/\mathbb{Z}$.*

Proof. The kernel K of this homomorphism is an additive subgroup of $\mathbb{R}$, and we distinguish three cases according as K is $\langle 0 \rangle$, discrete or dense. If $K = \langle 0 \rangle$ then $\mathcal{U} \cong \mathbb{R}$. If K is discrete, $\mathcal{U}$ is isomorphic to $\mathbb{R}/\mathbb{Z}$. If K is dense then, by continuity, $U(t) = I$ for all t. □

If $\mathcal{U} \cong \mathbb{R}/\mathbb{Z}$, the quantum walk is periodic. We will use $\mathbb{T}$ to denote $\mathbb{R}/\mathbb{Z}$ and we call the group $\mathbb{T}^m$ a *torus*. We will feel free to identify $\mathbb{T}$ with the multiplicative group of complex numbers of norm 1. A torus is a Lie group.

Why do we need to work with torii? If

$$U(t) = \sum_r e^{\mathrm{i}t\theta_r} E_r$$

we can factor the homomorphism from $\mathbb{R}$ to $\mathcal{U}$ into a map

$$t \mapsto (e^{\mathrm{i}t\theta_1}, \dots, e^{\mathrm{i}t\theta_m})$$

(from $\mathbb{R}$ to $\mathbb{T}^d$) followed by a homomorphism from $\mathbb{T}^d$ to $\mathcal{U}$. Both maps here are continuous, and the second map is injective. The problem of determining the image of the first map in $\mathbb{T}^m$ is important, and we wil take it up in Section sec:Kronecker.

8.3 Periods

Define the set $\mathrm{Per}(a)$ of periods of the graph X at a to be the set of times t such that $U(t)e_a$ is a scalar multiple of e_a. (Equivalently it is the set of times t such that e_a is an eigenvector for $U(t)$.) Clearly $\mathrm{Per}(a)$ is empty if X is not periodic at a.

8.3.1 Lemma. *If a is not an isolated vertex in X and X is periodic at a, then $\mathrm{Per}(a)$ consists of all integer multiples of some positive real number τ.*

Proof. Note that $\mathrm{Per}(a)$ is an additive subgroup of $\mathbb{R}$ and, as such, is either discrete or dense in $\mathbb{R}$.

If $\mathrm{Per}(a)$ is dense then there is a sequence of elements $(t_k)_{k\geq 0}$ of $\mathrm{Per}(a)$ with limit 0. We note that $U(t)$ is differentiable and so

$$\lim_{k\to\infty} \frac{1}{t_k}(U(t_k) - I)e_a = U'(0)e_a = \mathrm{i}Ae_a.$$

On the other hand, since t_k is a period we have that e_a is an eigenvector for $U(t_k) - I$ for each k, and the limit above must be a scalar multiple of e_a. Since a is not isolated, this is impossible and we conclude that $\mathrm{Per}(a)$ cannot be dense. Hence there is a unique positive real number τ such that $\mathrm{Per}(a)$ consists of all integral multiples of τ. □

We call τ the *minimum period* of X at a. (Corollary 7.6.2 provides a more explicit proof that the minimum period exists.)

If we use Q to denote the set of times at which we have perfect state transfer from a to b, then $2Q \subseteq \mathrm{Per}(a)$, and therefore if we have perfect state transfer at time t, then $2t$ is an integral multiple of τ.

8.3.2 Lemma. *Suppose u is a vertex in X with positive valency and X is periodic at u with minimum period σ. Then if there is perfect state transfer from u to v, there is perfect state transfer from u to v at time $\sigma/2$.*

Proof. Suppose we have uv-pst with minimum time τ. Then X is periodic at u, with minimum period σ (say).

If $\sigma < \tau$, then $U(\tau - \sigma)e_u = \gamma e_v$ for some γ and so τ is not minimal. Hence $\tau < \sigma$. Since X is periodic at u with period 2τ, we see that $\sigma \leq 2\tau$. If $\sigma < 2\tau$ then u is periodic with period dividing $2\tau - \sigma$ and so $\sigma \leq 2\tau - \sigma$, which implies that $\sigma \leq \tau$. We conclude that $\sigma = 2\tau$.

Thus if the minimum period of X at u is σ and there is perfect state transfer from u to v, then there is perfect state transfer from u to v at time $\sigma/2$ (and not at any shorter time). □

This result has the following important consequence, first noted by Kay [45, Section D].

8.3.3 Corollary. *If we have perfect state transfer in X from u to v and from u to w, then $v = w$.* □

It is worth noting that, even though the set of periods $\mathrm{Per}(a)$ is discrete, the corresponding phases need not be. If $U(t)e_a = \gamma e_a$, then

$$\gamma e_a = \sum_{r=0}^{d} e^{\mathrm{i}t\theta_r} E_r e_a.$$

Assume the graph is connected, E_0 corresponds to the largest eigenvalue, and so all of its entries are positive (according to Perron-Frobenius—see for instance [38, Chapter 8]). Multiplying both sides by E_0, we have

$$\gamma E_0 e_a = e^{\mathrm{i}t\theta_0} E_0 e_a,$$

thus $\gamma = e^{\mathrm{i}t\theta_0}$. If the graph is not connected (but a is not an isolated vertex), simply use the projector onto the eigenspace corresponding to the largest eigenvalue of the connected component containing a.

Consequently all integer powers of $e^{\mathrm{i}t\theta_0}$ are phases of a periodic time, and these powers are dense if and only if $t\theta_0/2\pi$ is irrational. It follows from Section 12.3 that cones over a regular graph provide examples where this ratio is indeed irrational.

8.4 Bounding the Minimum Period

It is possible to derive a lower bound on the minimum period in terms of the eigenvalues of X.

8.4.1 Lemma. *Suppose X is a graph with eigenvalues $\theta_1, \ldots, \theta_m$ in decreasing order and transition matrix $U(t)$. If x is a non-zero vector, then the minimum time τ such that $x^T U(\tau) x = 0$ is at least $\frac{\pi}{\theta_1 - \theta_m}$.*

Proof. Assume $\|x\| = 1$. We want

$$0 = x^T U(t) x = \sum e^{it\theta_s} x^T E_s x,$$

where the sum is over the eigenvalues θ_s such that $E_r x \neq 0$, i.e., over the eigenvalue support of x. Since

$$1 = x^T x = \sum x^T E_s x,$$

the right side is a convex combination of complex numbers of norm 1. When $t = 0$ these numbers are all equal to 1, and as t increases they spread out on the unit circle. If they are contained in an arc of length less than π, their convex hull cannot contain 0, and for small(ish) values of t, they lie in the interval bounded by $t\theta_1$ and $t\theta_m$. So for $x^T U_X(t) x$ to be zero, we need $t(\theta_1 - \theta_m) \geq \pi$, and thus we have the constraint

$$t \geq \frac{\pi}{\theta_1 - \theta_m}. \qquad \square$$

If $u \in V(X)$ and $x = e_u$, then this bound is tight for P_2 but not for P_3.

8.4.2 Lemma. *If X is a graph with eigenvalues $\theta_1, \ldots, \theta_m$, the minimum period of X at a vertex is at least $\frac{2\pi}{\theta_1 - \theta_m}$.*

Proof. We want

$$\gamma = \sum_r e^{i\theta_r t} (E_r)_{u,u},$$

where $\|\gamma\| = 1$, and for this to hold there must be integers $m_{r,s}$ such that

$$t(\theta_r - \theta_s) = 2m_{r,s}\pi.$$

This yields the stated bound. $\square$

In the previous lemma, θ_1 is the spectral radius of $A(X)$. However θ_m can be replaced by the least eigenvalue in the eigenvalue support of the relevant vertex. If the entries of x are non-negative, these comments apply to Lemma 8.4.1 too. For more bounds along the lines of the last two lemmas, go to [45, Section IIIC].

For vertex-transitive graphs we can specify the true period: if the eigenvalues are integers and 2^d is the largest power of 2 that divides the greatest common divisor of the difference of the eigenvalues, then the period is $\pi/2^{d-1}$.

It follows from Corollary 7.6.2 that the minimum period is at most 2π.

Let a be a vertex in X with dual degree m. Then the vectors $A^r e_a$ for $r = 0, \ldots, m$ form a basis for the walk module relative to a. If N is the matrix with these vectors as its columns then, since $\operatorname{col}(N)$ is A-invariant, there is a matrix B such that $AN = NB$. Consequently

$$U(t)N = N \exp(itB).$$

We can use the following to show that in certain cases, the phase factor γ arising in perfect state transfer is an m-th root of 1, for some m.

8.4.3 Lemma. *Suppose X is periodic at the vertex a at time t and with phase γ. If $\operatorname{tr}(B) = 0$ and the dual degree of a is m, then $\gamma^{m+1} = 1$.*

Proof. If $U(t)e_a = \gamma e_a$ then since $U(t)$ and A commute, $U(t)A^r e_a = \gamma A^r e_a$ and hence $U(t)N = \gamma N$. As the columns of N are linearly independent, we deduce that

$$\exp(itB) = \gamma I.$$

Now $\det(\exp(itB)) = 1$ for all t and $\det(\gamma I) = \gamma^{m+1}$. □

8.5 Kronecker's Theorem

Each continuous quantum walk determines a map $\mathbb{R} \to \mathbb{T}^m$:

$$t \mapsto (e^{\mathrm{i}t\theta_1}, \ldots, e^{\mathrm{i}t\theta_m})$$

The image of $\mathbb{R}$ under our first map is a subgroup of $\mathbb{T}^m$. From the theory of Lie groups we know that the closure of this group is isomorphic to $\mathbb{T}^\ell$, for some integer ℓ. The question we address here is simple to state, we want to know when $\ell = m$. We say that an element $(\theta_1, \ldots, \theta_m)$ is a *generator* of the torus $\mathbb{T}^m$ if the additive subgroup it generates is dense.

Our principal tool will be Kronecker's theorem. We first state its more general strong form.

8.5.1 Theorem. *Let $\lambda_1, \ldots, \lambda_n$ and $\theta_1, \ldots, \theta_n$ be arbitrary real numbers. For each δ in $\mathbb{R}_+$, there is t in $\mathbb{R}_+$ so that, for $k = 1, \ldots, n$*

$$|\lambda_k t - \theta_k| < \delta \pmod{2\pi}$$

if and only if, for all integers $\ell_1, \ldots, \ell_n$ such that $\ell_1\lambda_1 + \ldots + \ell_n\lambda_n = 0$, it also holds that

$$\ell_1\theta_1 + \ldots + \ell_n\theta_n \equiv 0 \pmod{2\pi}.$$

Proof. One direction is simple. If for any δ it is possible to find t satisfying (8.5.1), then we have, for all $k = 1, \ldots, n$,

$$-\delta < \lambda_k t - \theta_k - 2\pi m_k < \delta.$$

Given integers $\ell_1, \ldots, \ell_n$ so that $\ell_1\lambda_1 + \ldots + \ell_n\lambda_n = 0$, multiply each of these pairs of inequalities by the corresponding ℓ_k, and add all together, to recover

$$-\delta\left(\sum_{k=1}^{n} |\ell_k|\right) < -\left(\sum_{k=1}^{n} \ell_k\theta_k\right) - 2\pi\left(\sum_{k=1}^{n} \ell_k m_k\right) < \delta\left(\sum_{k=1}^{n} |\ell_k|\right).$$

Making $\delta \to 0$, it follows immediately that

$$\sum_{k=1}^{n} \ell_k\theta_k \equiv 0 \pmod{2\pi}.$$

For the other direction, define

$$f(t) = 1 + \mathrm{e}^{\mathrm{i}(\lambda_1 t - \theta_1)} + \ldots + \mathrm{e}^{\mathrm{i}(\lambda_n t - \theta_n)}.$$

Note that, for any δ there is a $t \in \mathbb{R}_+$ so that (8.5.2) holds if, and only if, $\sup_{t\in\mathbb{R}_+} |f(t)| = n + 1$. We will show that if this sup is not attained, then the condition on λs and θs cannot hold.

Let m be a positive integer. Then

$$f(t)^m = \sum_{\substack{a,\ell_1,\ldots,\ell_n\geq 0\\ a+\ell_1+\ldots+\ell_n=m}} \frac{m!}{a!\ell_1!\ldots\ell_n!}\left(\mathrm{e}^{\mathrm{i}(\lambda_1 t-\theta_1)}\right)^{\ell_1}\cdot\ldots\cdot\left(\mathrm{e}^{\mathrm{i}(\lambda_n t-\theta_n)}\right)^{\ell_n}$$
$$= \sum_{\substack{a,\ell_1,\ldots,\ell_n\geq 0\\ a+\ell_1+\ldots+\ell_n=m}} \frac{m!}{a!\ell_1!\ldots\ell_n!\cdot\mathrm{e}^{\mathrm{i}(\ell_1\theta_1+\ldots+\ell_n\theta_n)}}\ cdote^{\mathrm{i}t(\ell_1\lambda_1+\ldots+\ell_n\lambda_n)}.$$

By collecting terms, it is possible to write

$$f(t)^m = \sum_{\mu} a_\mu \mathrm{e}^{\mathrm{i}\mu t},$$

where each μ is unique and a_μ is a sum of multinomial coefficients multiplied by some complex phases. If

$$\ell_1\lambda_1+\ldots+\ell_n\lambda_n = \ell_1'\lambda_1+\ldots+\ell_n'\lambda_n$$

then, by hypothesis,

$$\ell_1\theta_1+\ldots+\ell_n\theta_n \equiv \ell_1'\theta_1+\ldots+\ell_n'\theta_n \pmod{2\pi}.$$

So the phases of the coefficients summing to each a_μ align, and, as a consequence,

$$\sum_\mu |a_\mu| = \sum_{\substack{a,\ell_1,\ldots,\ell_n\geq 0\\ a+\ell_1+\ldots+\ell_n=m}} \frac{m!}{a!\ell_1!\ldots\ell_n!} = (n+1)^m. \tag{8.5.1}$$

Now assume for the sake of contradiction that

$$\sup_{t\in\mathbb{R}_+} |f(t)| = \rho < n+1.$$

As a consequence,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T |f(t)^m|\mathrm{d}t \leq \rho^m.$$

However, from the expression of $f(t)^m$, it holds that, for each μ,

$$a_\mu = \lim_{T\to\infty}\frac{1}{T}\int_0^T f(t)^m\mathrm{e}^{-\mathrm{i}\mu t}\mathrm{d}t.$$

Thus

$$|a_\mu| \le \rho^m,$$

and, as the number of terms in the sum in Equation (8.5.1) is at most $(m+n)!/m!n!$, we have

$$\rho^m \cdot \frac{(m+n)!}{m! \cdot n!} \ge \sum_\mu |a_\mu| = (n+1)^m.$$

However, dividing by $(n+1)^m$ and taking the limit on both sides,

$$1 = \lim_{m\to\infty} \left(\frac{\rho}{n+1}\right)^m \cdot \frac{(m+n)!}{m! \cdot n!} \le \lim_{m\to\infty} \left(\frac{\rho}{n+1}\right)^m m^n = 0,$$

a contradiction. □

8.5.2 Theorem. *The element $(\alpha_1, \dots, \alpha_m)$ of $\mathbb{T}^m$ is a generator if and only if the numbers $1, \alpha_1, \dots, \alpha_m$ are linearly independent over the rationals.* □

If A is a symmetric matrix whose eigenvalues are linearly independent over $\mathbb{Q}$, this theorem implies that, for m in $\mathbb{Z}$, the vectors

$$(e^{in\theta_1}, \dots, e^{in\theta_m})$$

form a dense subgroup of $\mathbb{T}^m$. This is more than we will need: if $\Lambda(t)$ denotes the diagonal matrices of eigenvalues of $U_A(t)$, for our purposes it will suffice if the matrices $\Lambda(t)$ generate a dense subgroup of the torus, but Kronecker's theorem assures us that the matrices $\Lambda(n)$ are already dense.

On the other hand, in the cases of interest to us the matrix A is an integer matrix, whence it follows that the sum of its eigenvalues is an integer, and therefore these eigenvalues together with 1 are not linearly independent over $\mathbb{Q}$. However we will see that we can sometimes find a way around this difficulty, for example, if X is bipartite then it may be enough that the positive eigenvalues are linearly independent over $\mathbb{Q}$.

Bt way of example, we show that pretty good state transfers occus on P_5. The eigenvalues of P_5 are

$$\pm\sqrt{3},\ \pm 1,\ 0.$$

We number the eigenvalues so that there are exactly r eigenvalues greater than θ_r. You may check that

$$T = E_0 - E_1 + E_2 - E_3 + E_5$$

is the permutation matrix corresponding to the non-identity automorphism of P_5. Since 1 and $\sqrt{3}$ are linearly independent over $\mathbb{Q}$, we can choose t so that

$$(e^{it\theta_0}, e^{it\theta_1}) \approx (1, -1)$$

(where $\approx$ denotes "differs from by some specified small amount"). Since $\theta_4 = -\theta_0$ and $\theta_3 = -\theta_1$ it follows that at the same t we have $e^{it\theta_3} \approx -1$ and $e^{it\theta_3} \approx -1$. As $\theta_2 = 0$, we conclude that at time t,

$$(e^{it\theta_0}, e^{it\theta_1}, e^{it\theta_2}, e^{it\theta_3}, e^{it\theta_4}) \approx (1, -1, 1, -1, 1).$$

8.6 Dense Subgroups of $U(n)$

We show how we can use controllable pairs to generate dense subgroups of the unitary group. This treatment is taken from Godsil and Severini [39].

For our purposes, a Lie algebra is a vector space $\mathcal{L}$ of $n \times n$ matrices over a field ($\mathbb{R}$ or $\mathbb{C}$) such that if $A, B \in \mathcal{L}$, then

$$AB - BA \in \mathcal{L}$$

The term $AB - BA$ is known as the *Lie bracket* and is often denoted by $[A, B]$. We note that $[B, A] = -[A, B]$. If $\mathcal{L}$ is a Lie algebra, then the matrices

$$\{\exp(M) : M \in \mathcal{L}\}$$

form a group. Groups constructed in this way are *Lie groups*.

The set $\mathcal{L}$ of all $n \times n$ matrices is a real Lie algebra and the associated group is the group of all invertible real matrices. The subspace of $\mathcal{L}$ formed by the matrices with trace zero is a Lie algebra and its group is the group of real matrices with determinant one. The real skew symmetric matrices form the a Lie algebra, corresponding to the orthogonal group. The skew Hermitian matrices form a Lie algebra because

$$\begin{aligned}(AB - BA)^* &= B^*A^* - A^*B^* \\ &= (-B)(-A) - (-A)(-B) \\ &= BA - AB \\ &= -(AB - BA);\end{aligned}$$

the corresponding Lie group is the unitary group $U(n)$.

8.6.1 Lemma. *Let X be a graph and let z be the characteristic vector of a subset S of $V(X)$. Set $B = zz^T$. If (X, S) is controllable, the real Lie algebra generated by A and B is $\mathrm{Mat}_{n\times n}(\mathbb{R})$ and the real Lie algebra generated by iA and iL is the space of $n \times n$ skew-Hermitian matrices.*

Proof. We recall that if (X, S) is controllable, then the matrices

$$A^r B A^s, \quad (0 \le r, s \le n-1)$$

form a basis for the full matrix algebra. Let $\mathcal{L}$ be the Lie algebra generated by A and B; we aim to show that the elements of this basis lie in $\mathcal{L}$.

Note that

$$BA^rB = z(z^T A^r z)z^T = c_r B$$

where $c_r = z^T A^r z$. We prove by induction on k that $\mathcal{L}$ contains the matrices

$$A^{k-r} B A^r$$

for $r = 0, \dots, k$ and for all k. The case $k = 0$ is trivial, so assume inductively that $\mathcal{L}$ contains the above $k+1$ matrices. Then it contains the matrices

$$[A, A^{k-r}BA^r] = A^{k-r+1}BA^r - A^{k-r}BA^{r+1}$$

and hence it contains the partial sums $A^{k-r+1}BA^r - BA^{k+1}$ for each r.

In particular $\mathcal{L}$ contains $A^{k+1}B - BA^{k+1}$. Since

$$\begin{aligned}[B, A^{k+1}B - BA^{k+1}] &= BA^{k+1}B - A^{k+1}B^2 - B^2A^{k+1} + BA^{k+1}B \\ &= 2c_{k+1}B - c_0(A^{k+1}B + BA^{k+1}),\end{aligned}$$

we see that $\mathcal{L}$ contains both $A^{k+1}B - BA^{k+1}$ and $A^{k+1}B + BA^{k+1}$, and therefore it contains BA^{k+1}. Therefore $\mathcal{L}$ contains $A^{k-r+1}BA^r$ when $0 \le r \le k+1$.

Now we consider the real Lie algebra generated by the skew-Hermitian matrices iA and iB. Note that if M and N are symmetric matrices their commutator $[M, N]$ is skew symmetric and if M is symmetric and N skew symmetric, then $[M, N]$ is symmetric. We define the degree of a commutator as follows: A and B have degree zero and if M has degree zero and N has degree k then the degree of $[M, N]$ is $k+1$. Therefore commutators of even degree are symmetric and commutators of odd degree are skew symmetric. Since the intersection of the subspace of symmetric matrices with the subspace of skew symmetric matrices is the zero subspace, and since the commutators span the space of all matrices, it follows that the span of the odd commutators consists of all skew symmetric matrices. Given this it is not hard to verify that the Lie algebra generated by iA and iB has dimension n^2 and consists of all skew-Hermitian matrices. □

8.6.2 Theorem. *Let X be a graph and let z be the characteristic vector of a subset S of $V(X)$. Set $B = zz^T$. If (X, S) is controllable, the matrices in the sets*

$$\{\exp(itA) : t \in \mathbb{R}\}, \quad \{\exp(itB) : t \in \mathbb{R}\}$$

together generate a dense subgroup of the unitary group.

Proof. The two given sets are subgroups of unitary matrices and therefore the group they generate lies in $U(n)$. The closure Γ of this group is a Lie subgroup whose Lie algebra is generated by iA and iB. By the lemma, this Lie algebra consists of all skew-Hermitian matrices and therefore Γ is a Lie group locally isomorphic to $U(n)$. Therefore it is $U(n)$. □

We recall that if X is controllable, then A and J generate the full matrix algebra. The pair consisting of the path P_n and a vertex of degree one is controllable, this is in some sense the sparsest possible example.

If X is connected and Δ is the diagonal matrices of valencies if X, then J is a polynomial in $\Delta - A$. Therefore $\langle A, J\rangle \leq \langle A, \Delta\rangle$. If $\langle A, \Delta\rangle$ is the full matrix algebra then the arguments we have used above do not imply that iA and $i\Delta$ generate the Lie algebra of skew-Hermitian matrices. This might be true, but we cannot prove it.

8.7 Almost Periodic Functions

In Section 2.7, we saw that any continuous quantum walk is 'approximately recurrent': given $\tau > 0$ and $\epsilon > 0$ there is an integer k such that $\|U(k\tau) - I\| < \epsilon$. This leaves open the question as to how often the walk returns and, if it returns infinitely often, whether the time between returns bounded? In this section we give precise answers to this these questions.

A *trigonometric polynomial* is a finite sum

$$\sum_{r=1}^{m} a_R E^{\mathrm{i}\theta_r t}$$

where $a_1, \dots, a_m$ are complex and $\theta_1, \dots, \theta_m$ are real. The trigonometric polynomials form a complex vector space, in fact a complex algebra—the product of two trigonometric polynomials is a trigonometric polynomial. If A is the adjacency matrix of X and $U(t) = \exp(itA)$, then $U(t)_{a,b}$ is a trigonometric polynomial. For by the spectral decomposition,

$$U(t)_{a,b} = \sum_r e^{i\theta_r t}(E_r)_{a,b}.$$

The trigonometric polynomials form a subspace of the space of continuous functions in $\mathbb{R}$ and so, given a norm on continuous functions, we may take its completion. If we choose the norm $\|\cdot\|_\infty$, the completion we get is the space of *almost periodic functions*. Since it is a completion, this is a Banach space and it is not too hard to show that it is actually a Banach algebra—the product of two almost periodic functions is almost periodic.

Almost periodic functions are 'approximately recurrent'; we set about explaining what we mean by this.

A real number τ is an *ϵ-period* for a complex-valued function $f(t)$ if, for all t,

$$\|f(t+\tau) - f(t)\| < \epsilon.$$

A sequence of real numbers is *relatively dense* if there is a real number L such that every real interval of length L contains at least one element of the sequence.

8.7.1 Theorem. *A complex-valued function $f(t)$ is almost periodic if it is continuous and, for each positive real number ϵ, there is a relatively dense set of ϵ-periods for f.* □

Note that if

$$f(t) = \sum_r a_r e^{i\theta_r t}$$

is a trigonometric polynomial, then the map

$$f \mapsto \sum_r |a_r|$$

is a norm on the space of trigonometric polynomials; the closure of the trigonometric polynomials relative to this norm gives a proper subspace of the space of almost periodic functions. In fact there are a number of classes of almost-periodic functions.

We treat some applications of almost-periodic functions to continuous quantum walks. There are two slightly different approaches. One is to take the view that $U(t)$ is an almost-periodic function taking values in the algebra of $n \times n$ complex matrices. The second is to work with the entries of $U(t)$, which are almost periodic according to our definition.

8.7.2 Theorem. *For any graph X and positive ϵ, there is a relatively dense set of times $\mathcal{P}$ such that $\|U(t) - I\| < \epsilon$ for all t in $\mathcal{P}$.*

Proof. Set $U_0 = U(t_0)$. Then

$$\operatorname{tr}((U(t) - U_0)^*(U(t) - U_0)) = \operatorname{tr}(2I - U(t)^*U_0 - U_0^*U(t))$$

is an almost periodic function that is zero at t_0. Hence there is a relatively dense subset $\mathcal{P}$ of $\mathbb{R}$ such that $\|U(t) - U(t_0)\| < \epsilon$ for all t in $\mathcal{P}$. Since $U(0) = I$, the theorem follows. □

If $\|U(\tau) - I\| < \epsilon$, then

$$\begin{aligned}\|U(t+\tau) - U(t)\| &= \|(U(\tau) - I)U(t)\| \\ &\le \|U(\tau) - I\|\,\|U(t)\| \\ &= \|U(\tau) - I\|.\end{aligned}$$

Thus if $\|U(\tau) - I\| < \epsilon$, then τ is an ϵ-period for $U(t)$. Note that Theorem 2.7.2 implies the existence of ϵ-periods, the problem we have addressed here is to get a relatively dense set.)

8.8 Means

8.8.1 Theorem. *If f is almost periodic then*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(t)\,dt$$

exists. □

If $f(t) = U(t)_{a,b}$, then

$$\mathcal{M}(f) = (E_0)_{a,b}.$$

(With the understanding that $E_0 = 0$ if 0 is not an eigenvalue of X.)

We denote the limit in the theorem by $\mathcal{M}(f)$, and call it the *mean* of f.

See Corollary 3.1 to Theorem 3.4 in Constantin Corduneanu "Almost Periodic Oscillations and Waves" (Springer, New York) 2008 for existence of the mean. See Proposition 3.15 in the same source for the following.

8.8.2 Theorem. *The map $f \mapsto \mathcal{M}(|f|)$ is a norm on the space of almost-periodic functions.* □

8.8.3 Corollary. *If f is a real non-zero almost-periodic function and $\mathcal{M}(f) = 0$, then f changes sign.*

Proof. If f does not change sign, then we may assume without loss that $f \geq 0$. Now

$$0 = \mathcal{M}(f) = \mathcal{M}(|f|)$$

and consequently f is identically zero. □

Of course if f changes sign, then it follows that its zeros form a relatively dense subset of $\mathbb{R}$. Our next result shows that an almost periodic function assumes its mean value on a relatively dense subset of $\mathbb{R}$.

8.8.4 Corollary. *If f is real and almost periodic and $\mathcal{M}(f) = \hat{f}$, then $\{t : f(t) = \hat{f}\}$ is a relatively dense subset of $\mathbb{R}$.*

Proof. Apply the above to $f - \hat{f}$. □

8.8.5 Lemma. *If A is invertible then $\mathcal{M}(U(t)) = 0$, and otherwise $\mathcal{M}(U(t)) = E_0$.* □

Proof. We have

$$U(t) = \sum_r (\cos(\theta_r t) + i \sin(\theta_r t)) E_r,$$

since $\mathcal{M}(\sin(\theta_r t)) = 0$ and since $\mathcal{M}(\cos(\theta_r t)) = 0$ is $\theta_r \neq 0$, the result follows. □

8.9 Zeros of Transition Functions

This section is unpublished joint work of the second author with Tino Tamon and Hisao Tamaki. It is motivated by the plots of $M(t)_{a,b}$, which show that this function is often zero, or very close to zero. The difficulty is to decide which. The following lemma gives a sufficient condition.

8.9.1 Lemma. *Suppose a and b are vertices in the graph X. If a and b are at odd distance in X, or if X is bipartite and 0 is not eigenvalue of X, then the zeros of $U(t)_{a,b}$ form a relatively dense subset of $\mathbb{R}$.*

Proof. Suppose $d = \mathrm{dist}(u, v) > 0$. Since

$$U(t)_{u,v} = \sum_k \frac{(it)^k}{k!}(A^k)_{u,v}$$

We see that 0 is a zero of the function $U(t)_{u,v}$ with multiplicity exactly d. Since zeros of odd multiplicity of a function f are stable under small perturbations of f, and since $U(t)_{a,b}$ is almost periodic, it follows that it has a relatively dense set of zeros.

Now assume X is bipartite and 0 is not an eigenvalue of A. Then

$$U(t)_{a,b} = \sum_r e^{i\theta_r t}(E_r)_{u,v}.$$

If d is odd, we are already done. If d is even, then

$$(E_\lambda)_{u,v} = (E_{-\lambda})_{u,v}$$

and therefore

$$U(t)_{a,b} = 2 \sum_{r:\theta_r>0} (E_r)_{u,v} \cos(\theta_r t).$$

Thus the mean of $U(t)_{a,b}$ is 0, and again this function has a relatively dense set of zeros. □

We note that if $X = K_n$ and $n > 4$, then $U(t)_{u,u}$ is never zero.

For P_5 (bipartite, eigenvalues $\{\pm\sqrt{3}, \pm 1, 0\}$) you may show that $U(t)_{0,4}$ is never zero when $t > 0$. (This is not obvious from the plot of $M(t)_{0,4}$ shown on the next page.)

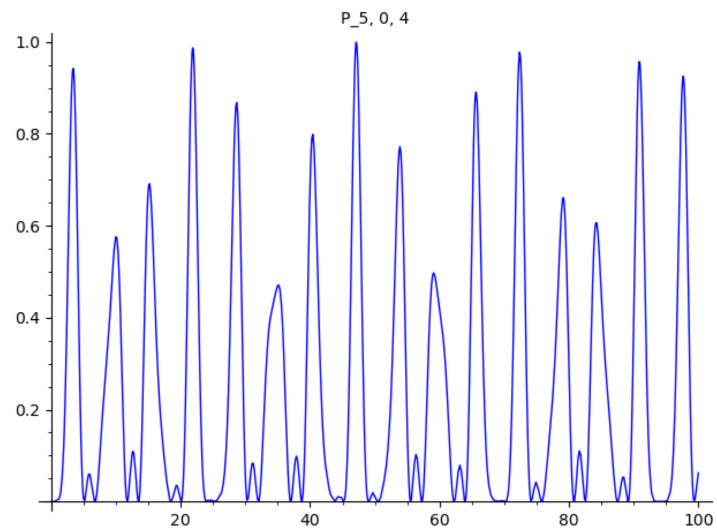

Figure 8.1: P_5: $M(t)_{0,4}$

Notes

unitary group kronecker almost periodic: References. Not always physically meaningful

Exercises

8-1. Show that $U_{P_5}(t)_{0,4} = 0$ if and only if $t = 0$.

Chapter 9

Real State Transfer

We have seen the the existence of perfect state transfer on a graph has a number of consequences. To summarize, if there is pst from a to b at time t, then:

(a) There is pst from b to a at time t.

(b) $D_a(2t) = D_a$.

(c) If θ_k, θ_ℓ, θ_r and θ_s lie in the eigenvalue support of a and $\theta_k \neq \theta_\ell$, then

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}$$

(d) The vertices a and b are strongly cospectral.

If the initial state of a continuous quantum walk on a graph X is given by a density matrix D, then the state $D(t)$ at time t is given by

$$D(t) = U(t)DU(-t).$$

We have perfect state transfer from a to b if $D_a(t) = D_b$ at some time t. In this chaper we will see that most of the consequences of perfect state transfer follow simply from the assumption that the density matrices D_a and D_b are real.

We will also see that interesting things happen if we assume that the entries of D and $D(t)$ are algebraic numbers.

9.1 Real State Transfer

A state is *real* if its density matrix is real. We recall that we have perfect state transfer at time t from a density matrix P to a density matrix Q if $P(t) = Q$. We say that we have *pretty good state transfer* from a state P to Q if for each positive real number ϵ there is a time t_ϵ such that $\|(U(t)PU(t) - Q)\| < \epsilon$.

We define the *eigenvalue support of a density matrix* P to be the set of pairs (θ_r, θ_s) such that $E_rPE_s \neq 0$. (This definition extends the one given in the introduction to density matrices not of the form D_a.) We say that the eigenvalue support of P satisfies the ratio condition if, for each two pairs of distinct eigenvalues in the eigenvalue support of P, we have

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}.$$

Note that if P is pure, that is, $P = xx^*$ for some unit vector x, then $E_rPE_s = 0$ if and only if E_rx or E_sx is zero. (In this case we could define the eigenvalue support to be the the set of eigenvalues θ_r such that $E_rPE_r \neq 0$, which what we do elsewhere.)

9.1.1 Theorem. *Let $U(t)$ be the transition matrix corresponding to a graph X. If P is a real density matrix, there is a positive time t such that $U(t)PU(-t)$ is real if and only if the eigenvalue support of P satisfies the ratio condition.*

Proof. We have

$$P^{(t)} = \sum_{r,s} e^{it(\theta_r - \theta_s)} E_rPE_s$$

and therefore the imaginary part of $P^{(t)}$ is

$$\sum_{r,s} \sin(t(\theta_r - \theta_s))E_rPE_s.$$

The non-zero matrices E_rPE_s are linearly independent, and therefore the imaginary part of $P^{(t)}$ is zero if and only if $\sin(t(\theta_r - \theta_s)) = 0$ whenever $E_rPE_s \neq 0$. Hence if (θ_r, θ_s) lies in the eigenvalue support of P then there is an integer $m_{r,s}$ such that $t(\theta_r - \theta_s) = m_{r,s}\pi$. □

9.1.2 Lemma. *Let P be a real density matrix. If $P(t)$ is real, then $P(2t) = P$ and $U(2t)$ commutes with P and Q.*

Proof. If $U(t)PU(-t) = Q$ where Q is real, then taking complex conjugates yields

$$U(-t)PU(t) = Q$$

and consequently $P = U(t)QU(-t)$. It follows at one that $U(2t)$ commutes with P. □

9.1.3 Lemma. *If A is real and symmetric and we have state transfer at t between real density matrices P and Q, then*

(a) $E_r P E_r = E_r Q E_r$.

(b) If $t(\theta_r - \theta_s)$ is not a multiple of π then $E_r P E_s = E_r Q E_s = 0$.

(c) Otherwise $E_r P E_s = \pm E_r Q E_s$.

Proof. If A is real and symmetric then the idempotents E_r are real and symmetric. Assume

$$Q = U(\tau)PU(-\tau) = \sum_{r,s} e^{i\tau(\theta_r - \theta_s)} E_r P E_s.$$

If we multiply this expression on the left by E_r and on the right by E_s, then

$$E_r Q E_s = e^{i\tau(\theta_r - \theta_s)} E_r P E_s$$

and, since all matrices here are real, $e^{it(\theta_r - \theta_s)}$ must be real.

Since $\sum_{r,s} E_r P E_s = P$, we see that if A is real and there is pst from P to Q, there are signs $\epsilon_{r,s} = \pm 1$ such that

$$Q = \sum_{r,s} \epsilon_{r,s} E_r P E_s.$$ □

Consider the rank-one case. If $P = uu^T$ then $E_r uu^T E_s = 0$ if and only if $E_r u = 0$ or $E_s u = 0$. Hence the constraint in (b) gives a constraint on the eigenvalue support of u. (In fact this is the usual ratio condition, so (b) generalizes this.)

In the rank-one case, if $E_r P E_s = 0$ then either $PE_r = 0$ or $PE_s = 0$. So the known results for pure states will extend to the case where, for all r and s,

$$E_r P E_s = 0 \iff E_r P E_r = 0 \text{ or } E_s P E_s = 0.$$

Note that $E_rPE_r = 0$ if and only if $P^{1/2}E_r = 0$.

If $E_rPE_s = 0$ whenever $r \neq s$, then

$$P = \sum_r E_rPE_r$$

and $PA = AP$; thus $U(t)PU(-t) = P$ for all t.

9.2 Pretty Good State Transfer

We have *pretty good state transfer* from a state P to a state Q if, for each $\epsilon > 0$, there is a time t such that

$$\|U(t)PU(-t) - Q\| < \epsilon.$$

Since the complex conjugate of

$$U(t)PU(-t) - Q$$

is

$$U(-t)PU(t) - Q = U(-t)\left(P - U(t)QU(-t)\right)U(t)$$

and since $U(t)$ is unitary,

$$\|U(t)PU(-t) - Q\| = \|P - U(t)QU(-t)\|.$$

Hence if we have pretty good state transfer from P to Q, then we have pretty good state transfer from Q to P.

9.2.1 Lemma. *Suppose A is real and we have pretty good state transfer from P to Q. Then $E_rPE_s = \pm E_rQE_s$ (for all r and s) and $E_rPE_r = E_rQE_r$.*

Proof. By assumption there is an increasing sequence of times $(t_k)_{k\geq 0}$ such that

$$U(t_k)PU(-t_k) \to Q$$

as $t_k \to \infty$. Hence

$$e^{i(\theta_r - \theta_s)t_k} E_rPE_s \to E_rQE_s$$

as $t_k \to \infty$. Since E_rPE_s and E_rQE_s are real, the result follows. □

9.2.2 Corollary. *If A is real and P is real, there are only finitely many real density matrices Q for which there is pretty good state transfer from P to Q.*

Proof. Since $Q = \sum_{r,s} E_r Q E_s$ it follows that $Q = \sum_{r,s} \epsilon_{r,s} E_r P E_s$, where $\epsilon_{r,s} = \pm 1$. □

9.3 Algebras

Because they are trace-orthogonal, the non-zero matrices $E_r P E_s$ are linearly independent. The "off-diagonal" terms $E_r P E_s$ are nilpotent, indeed the matrices

$$E_r P E_s, \quad (r < s)$$

generate a nilpotent algebra, where the product of any two elements is zero. The "diagonal" terms $E_r P E_r$ generate a commutative semisimple algebra; their sum is the orthogonal projection of P onto the commutant of A (see [23] for further details).

Since $U(t)$ is a linear combination of the spectral idempotents of A, it is a polynomial in A and therefore, for each t we that $P(t) in \langle A, P\rangle$. In consequence

$$\langle P(t), A\rangle = \langle P, A\rangle$$

for all t.

9.3.1 Lemma. *If we have pretty good state transfer from P to Q, then $\langle A, P\rangle = \langle A, Q\rangle$.* □

Proof. The algebra $\langle A, P\rangle$ is closed and as Q is a limit of a sequence of matrices in it, it follows that $Q \in \langle A, P\rangle$. If we have pretty good state transfer from P to Q, then as we noted st the beginning of Section **??**, there is pretty good state transfer from Q to P and so $\langle A, P\rangle = \langle A, Q\rangle$. □

If $\langle A, P\rangle$ is the full matrix algebra, we say that P is *controllable*. If P is real and $P(t)$ is real, then $U(2t)$ commutes with A and P. If P is also controllable it follows that $U(2t)$ must be a scalar matrix, say $U(2t) = \zeta I$. Since $\det(U(t)) = 1$, we have $\zeta^{|V(X)|} = 1$ and therfore ζ is a root of unity.

9.4 Timing

9.4.1 Lemma. *Let P be a density matrix and let S be given by*

$$S := \{\sigma : U(\sigma)PU(-\sigma) = P\}.$$

Then there are three possibilities:

(a) $S = \emptyset$.

(b) There is a positive real number τ and S consists of all integer multiples of τ.

(c) S is a dense subset of $\mathbb{R}$ and $U(t)PU(-t) = P$ for all t.

Proof. Suppose $S \neq \emptyset$. Then S is an additive subgroup of $\mathbb{R}$ and there are two cases. First, S is discrete and consists of all integer multiples of its least positive element. Second, S is dense in $\mathbb{R}$ and there is sequence of positive elements $(\sigma_i)_{i\geq 0}$ with limit 0. Since for small values of t we have

$$U(t) \approx I + itA$$

it follows that $AP = PA$ and $U(t)PU(-t) = P$ for all t. □

If $U(t)PU(-t) = P$ when $t = \tau > 0$, but not for all t, we say that P is *periodic* with period τ. If a density matrix is periodic, it has a well defined minimum period. If there is perfect state transfer from P to Q, then P and Q are both periodic with the same minimum period.

9.4.2 Lemma. *Suppose P and Q are distinct real density matrices. If there is perfect state transfer from P to Q, then P is periodic and if the minimum period of P is σ, then pst occurs at time $\sigma/2$.*

Proof. Suppose we have pst from P to Q and define

$$T := \{t : U(t)PU(-t) = Q\}$$

Assume that the minimum period of P is σ. If $t \in T$ then P is periodic with period $2t$ and so T is a coset of a discrete subgroup of $\mathbb{R}$. Also $T = -T$. Let τ be the least positive element of T. Then $2\tau \geq \sigma$ and thus

$$\tau \geq \frac{1}{2}\sigma.$$

If $\tau \geq \sigma$ then $\tau - \sigma \in T$ and since τ is not a period, $\tau < \sigma$. As σ must divide 2τ, it follows that $\tau = \sigma/2$. □

9.4.3 Corollary. *For any real density matrix P, there is at most one real density matrix Q such that there is perfect state transfer from P to Q.* □

9.4.4 Lemma. *Suppose we have pst from P to Q at time t and that $\theta_1, \ldots, \theta_m$ are the distinct eigenvalues of A in nonincreasing order. If* $\operatorname{tr}(PQ) = 0$ *then*

$$t \geq \frac{\pi}{\theta_1 - \theta_m}.$$

Proof. Since $P \succcurlyeq 0$, it has a unique positive semidefinite square root which we denote by $P^{1/2}$. We calculate that

$$\begin{aligned}\langle P, U(t)PU(-t)\rangle = \operatorname{tr}(PU(t)PU(-t)) &= \operatorname{tr}(P^{1/2}U(t)P^{1/2}P^{1/2}U(-t)P^{1/2}) \\ &= \operatorname{tr}((P^{1/2}U(t)P^{1/2})(P^{1/2}U(t)P^{1/2})^*),\end{aligned}$$

and from this it follows that $\langle P, U(t)PU(-t)\rangle = 0$ if and only if

$$P^{1/2}U(t)P^{1/2} = 0.$$

Now

$$P^{1/2}U(t)P^{1/2} = \sum_r e^{it\theta_r} P^{1/2}E_rP^{1/2};$$

here the matrices $P^{1/2}E_rP^{1/2}$ are positive semidefinite and hence their eigenvalues are real and non-negative.

When t is small, the eigenvalues of $U(t)$ on a small arc of the unit circle in the complex plane, and this arc contains 1. If the eigenvalues of $U(t)$ lie on arc of the unit circle with length less than π, then $\sum_r e^{it\theta_r} P^{1/2}E_rP^{1/2}$ cannot be zero.

Therefore if P and $U(t)PU(-t)$ are orthogonal, then $t(\theta_1 - \theta_m) \geq \pi$. □

Note that in this lemma we do not need P and Q to be real.

9.5 Periodicity and Eigenvalues

A state D is periodic (relative to the continuous walk on X), if there is non-zero time τ such that

$$D(\tau) = D.$$

Theorem 9.1.1 tells us that if D and $D(\tau)$ are both real, the eigenvalues of the Hamiltonian satisfy the ratio condition. We derive a version of this result for periodic states.

9.5.1 Theorem. *Let D be a rational state. If D is periodic at some time τ, there is a square-free integer Δ such that if (r,s) lies in the eigenvalue support of D, then $(\theta_r-\theta_s)$ is an integer multiple of $\sqrt{\Delta}$.*

Proof. We have

$$D(t)=\sum_{r,s} e^{\mathrm{i}\tau(\theta_r-\theta_s)}E_rDE_s$$

and, since $\sum E_r=I$,

$$D=\sum_{r,s} E_rDE_s.$$

Therefore

$$E_kDE_\ell=E_kD(t)E_\ell=e^{\mathrm{i}\tau(\theta_k-\theta_\ell)}E_kDE_\ell$$

which yields that

$$e^{\mathrm{i}\tau(\theta_k-\theta_\ell)}=1$$

whenever $E_kDE_\ell\neq 0$. If $e^{\mathrm{i}\tau(\theta_k-\theta_\ell)}=1$, there is an integer $m_{k,\ell}$ such that $\tau(\theta_k-\theta_\ell)=2m_{k,\ell}\pi$ and hence if (r,s) and (k,ℓ) lie in the eigenvalue support of D, we have the ratio condition:

$$\frac{\theta_r-\theta_s}{\theta_k-\theta_\ell}\in\mathbb{Q}.$$

Let Γ denote the Galois group of the splitting field $\mathbb{K}$ of the characteristic polynomial of X over $\mathbb{Q}$. If M is a matrix over $\mathbb{K}$ and $\gamma\in\Gamma$, let M^γ be the result of applying γ to each entry of M. If $\gamma\in\Gamma$ and E is a spectral idempotent of A with eigenvalue θ, then

$$AE^\gamma=(AE)^\gamma=(\theta E)^\gamma=\theta^\gamma E^\gamma,$$

which implies that E^γ is a spectral idempotent of A.

Let S denote the eigenvalue support of D. If $E_rDE_s\neq 0$, then since D is rational, $(E_r)^\gamma D(E_s)^\gamma\neq 0$, and therefore the set

$$\{(\theta_r,\theta_s):(r,s)\in S\}$$

is closed under γ. Consequently if $(k,\ell)\in S$,

$$\prod_{(r,s)\in S}\frac{\theta_k-\theta_\ell}{\theta_r-\theta_s}=\frac{(\theta_k-\theta_\ell)^{|S|}}{\prod_{(r,s)\in S}(\theta_r-\theta_s)}.$$

The product

$$\prod_{(r,s)\in S} (\theta_r - \theta_s)$$

is invariant under Γ, and this it is an integer; given the ratio condition, this implies that

$$(\theta_k - \theta_\ell)^{|S|} \in \mathbb{Q}.$$

Arguing as in the proof of Theorem 7.6.1, we deduce that $(\theta_r - \theta_s)^2$ is an integer and that the integers

$$(\theta_r - \theta_s)^2, \quad (r,s) \in S,$$

all have the same square-free part. □

9.6 Periodic Subsets

If $S \subseteq V(X)$, define D_S to be the diagonal matrix with $(D_S)_{a,a} = 1$ if $a \in S$ and $(D_S)_{a,a} = 0$ otherwise. Then $|S|^{-1}D_S$ is a density matrix and we mat refer to it as a *subset state*. In fact we will abuse notation and refer to D_S as a state. A subset S of $V(X)$ is *periodic* if there is a time τ such that $U(\tau)$ and D_S commute. (Thus periodic vertices are one-element subset states.)

The matrix D_S is idempotent, and represents orthogonal projection onto the subspace

$$\operatorname{span}\{e_a : a \in S\}.$$

Accordingly a matrix M commutes with D_S if and only if this subspace is M-invariant. In particular S is periodic at time τ if and only if, for each vertex b in S,

$$U(\tau)e_b \in \operatorname{span}\{e_a : a \in S\}.$$

Assume S is a subset of $V(X)$. If M is a square matrix indexed by $V(X)$, we use $M_{S,S}$ to denote the submatrix of M with rows and columns indexed by elements of S. We define the *induced adjacency algebra* of X on S to be the matrix algebra generated by the matrices

$$(E_r)_{S,S}, \qquad r = 1, \dots, m.$$

We denote it by $\mathcal{A}(S)$ and observe that it is isomorphic to the algebra generated by the $n \times n$ matrices

$$D_S E_r D_S, \qquad r = 1, \dots, m.$$

(We may not always distinguish between these two representations.) It is an easy exercise to verify that $\mathcal{A}(S)$ is also generated by the matrices

$$(A^k)_{S,S}, \qquad k \geq 0.$$

From Corollary 4.5.2 we see that if S is a parallel subset of $V(X)$, then $\text{rk}((E_r)_{S,S}) \leq 1$ for each r. □

9.6.1 Lemma. *If the subset S of $V(X)$ is periodic relative to the continuous walk on X at time τ, then $U(\tau)_{S,S}$ belongs to the center of the induced algebra on S.* □

Proof. Since $U(\tau)$ is block diagonal and commutes with E_r for each r, it follows that $(U(\tau)_{S,S})$ commutes with $(E_r)_{S,S}$ for each r. □

9.7 Algebraic States

We say that a state with density matrix D is *algebraic* if the entries of D are algebraic numbers. Clearly the vertex states D_a are algebraic; we give a second class of examples.

Suppose D is a pure state. Then $D(t)$ is pure for all t. If $D = zz^*$, then $D(t) = ww^*$, where $w = U(t)z$. We say that a matrix or vector is *flat* if all its entries have the same absolute value. We see that a vector w is flat if and only the diagonal entries of ww^* are all equal. (Note that these entries are non-negative and real.)

We say that a quantum walk has *uniform mixing relative to a pure state* D if there is a time t such that

$$D(t) \circ I = \frac{1}{n} I.$$

The walk has *uniform mixing* if it admits uniform mixing relative to each vertex. In many of the cases where uniform mixing is known to occur, the underlying graph is vertex transitive, and then uniform mixing occurs if and only if uniform mixing relative to a vertex occurs. The only examples we know of graphs that are not regular and admit uniform mixing are the complete bipartite graph $K_{1,3}$ and its Cartesian powers. If $n \geq 2$, the stars $K_{1,n}$ admit uniform mixing relative to the vertex of degree n.

9.7.1 Lemma. *Assume X is bipartite and $a \in V(X)$. If the quantum walk on X has uniform mixing at time relative to the pure state D_a, then $D_a(t)$ is algebraic.*

9.7.2 Theorem. *If the density D is algebraic and, for some t, the density $D(t)$ is algebraic, then the ratio condition holds on the eigenvalue support of D.*

Proof. We have

$$D(t) = \sum_{r,s} e^{it(\theta_r - \theta_s)} E_r D E_s$$

The matrices $E_r D E_s$ are pairwise orthogonal, and so, for all r and s,

$$\langle D(t), E_r D E_s \rangle = e^{it(\theta_r - \theta_s)} \langle E_r D E_s, E_r D E_s \rangle.$$

The entries of the spectral idempotents are algebraic, and if the entries of D and $D(t)$ are algebraic, then the values of the two inner products in the above identity are algebraic numbers.

It follows that $e^{it(\theta_r - \theta_s)}$ must be algebraic, for all r and s. Now if $k \neq \ell$, then

$$e^{it(\theta_r - \theta_s)} = \left(e^{it(\theta_k - \theta_\ell)} \right)^{\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell}} .$$

The Gelfond-Schneider theorem tells us that if α and β are algebraic numbers and $\alpha \neq 0, 1$ and β is irrational, then α^β is transcendental, whence we deduce that if D and $D(t)$ are algebraic, then the ratios

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell}$$

are all rational.

We say that the continuous quantum walk on X is *periodic at a* if there is a time τ such that $D_a(\tau) = D_a$.

9.7.3 Corollary. *If X is bipartite and there is uniform mixing on X relative to the vertex a, then X is periodic at a and the eigenvalue support of a consists of integer multiples of Δ, where $\Delta^2 \in \mathbb{Z}$.* □

9.8 Fractional Revival

Having seen that perfect state transfer is rare, it is natural to look for relaxations of the idea. We have already considered one, pretty good state transfer. We introduce a second variant.

If a and b are two vertices in X, we say that we have *fractional revival* on $\{a,b\}$ if there is a time t and scalars α and β such that

$$U(t)e_a = \alpha e_a + \beta e_b.$$

When the values of α and β are significant, we may say that we have fractional (α,β)-revival. As $U(t)$ is unitary must have $|\alpha|^2 + |\beta|^2 = 1$. (It might appear that we should have "fractional revival from a to b"; the reason for the given wording will become clear shortly.) If $\beta = 0$, then fractional revival reduces to periodicity at a, and if $\alpha = 0$, we have perfect state transfer. We say we have *proper* fractional revival if $\beta \neq 0$. (This condition excludes the case that the vertex a is periodic.)

To provide an example, we consider the graph $K_2 \otimes K_n$. If $n \geq 3$, this has diameter three and, moreover, it is antipodal—for each vertex there is a unique vertex at distance three.

9.8.1 Lemma. *At time $2\pi/n$, there is fractional revival between antipodal vertices in $K_2 \times K_n$.*

Proof. From Equation (12.6.1), we have

$$U_{K_2\times Y}(t) = \frac{1}{2}\begin{pmatrix} U_Y(t) + U_Y(-t) & U_Y(t) - U_Y(-t) \\ U_Y(t) - U_Y(-t) & U_Y(t) + U_Y(-t) \end{pmatrix}.$$

Now if we set

$$E_0 = \frac{1}{n}J, \quad E_1 = I - E_0,$$

then

$$U_{K_n}(t) = e^{-\mathrm{i}t}(e^{n\mathrm{i}t}E_0 + E_1), \quad U_{K_m}(-t) = e^{\mathrm{i}t}(e^{-n\mathrm{i}t}E_0 + E_1)$$

Set $t = 2\pi/n$. Then $e^{nit} = 1$ and

$$\begin{aligned} U_{K_n}(t) + U_{K_n}(-t) &= 2\cos(2\pi/n)I, \\ U_{K_n}(t) - U_{K_n}(-t) &= 2\sin(2\pi/n)I, \end{aligned}$$

which in turn implies that

$$U_{K_2 \otimes K_n}(2\pi/n) = \begin{pmatrix} 2\cos(2\pi/n) & 2\sin(2\pi/n) \\ 2\sin(2\pi/n) & 2\cos(2\pi/n) \end{pmatrix} \otimes I_n. \qquad \square$$

We describe another class of examples using the Cartesian product.

9.8.2 Lemma. *Assume that the quantum walk on X is periodic at time τ, where $\tau < \pi/2$. Let $V(K_2) = \{1,2\}$. Then for each vertex u in X, the Cartesian product $X \,\square\, K_2$ admits fractional revival on $\{(u,1),(u,2)\}$ at time τ.*

Proof. Recall that

$$U_{X \square K_2}(t) = U_X(t) \otimes U_{K_2}(t).$$

This describes a setup where Alice is running the continuous walk on X (in her lab) and Bob the walk on K_2 in his. If the initial state is $e_u \otimes e_1$, then at time τ there is a complex scalar γ such that the state is

$$U_X(\tau)e_u \otimes U_{K_2}(\tau)e_1 = \gamma e_u \otimes U_{K_2}(\tau)e_1.$$

Since τ is less than the period of the walk on K_2, we see that

$$U_{K_2}(\tau) = \alpha e_1 + \beta e_2$$

with $\alpha\beta \neq 0$. $\square$

This construction works in part because K_2 admits fractional revival at any time that is not an integer multiple of $\pi/2$.

The path P_4 admits fractional revival between its vertices of valency 1 at time $2\pi/\sqrt{5}$ (and hence between its vertices of degree two at the same time). Proving this requires more effort, so we leave it as an exercise.

9.9 Symmetry

We work towards showing that fractional revival is symmetric in the vertices involved.

9.9.1 Lemma. *If $U(t)e_a = \alpha e_a + \beta e_b$, and $\beta \neq 0$ then*

$$U(t)e_b = \beta e_a - \frac{\overline{\alpha}\beta}{\overline{\beta}} e_b.$$

If $U(t)e_a = \alpha e_a + \beta e_b$, then

$$e_a = \alpha U(-t)e_a + \beta U(-t)e_b$$

and, taking complex conjugates, this implies that

$$e_a = \bar{\alpha}U(t)e_a + \overline{\beta}U(t)e_b.$$

Therefore

$$e_a = \bar{\alpha}(\alpha e_a + \beta e_b) + \overline{\beta}U(t)e_b$$

and (if $\beta \neq 0$), this yields

$$U(t)e_b = \overline{\beta}^{-1}((1 - \bar{\alpha}\alpha)e_a - \bar{\alpha}\beta e_b)$$

and, as $1 - \alpha\bar{\alpha} = \beta\overline{\beta}$, the lemma follows. □

This shows that admitting fractional revival is a property of the pair of vertices, not of the ordered pair. Hence we have:

9.9.2 Lemma. *There is fractional revival on $S = \{a, b\}$ if and only if S is periodic.* □

We note another useful consequence of Lemma 9.9.1.

9.9.3 Corollary. *If we have proper fractional revival on a and b, then a and b are parallel with the same eigenvalue support.*

Proof. If $U(t)e_a = \alpha e_a + \beta e_b$, then

$$(U(t) - \alpha I)e_a = \beta e_b$$

If E_r is a spectral idempotent of A with eigenvalue θ_r, then multiplying both sides of this equation by E_r yields that

$$(e^{\mathrm{i}\theta_r t} - \alpha)E_r e_a = \beta E_r e_b.$$

As $\beta \neq 0$, we see that $|\alpha| < 1$ and so $e^{\mathrm{i}\theta_r t} - \alpha \neq 0$. □

This result implies, among other things, that if we have fractional revival on $\{a, b\}$, then $\mathrm{Aut}(X)_a = \mathrm{Aut}(X)_b$. (See Lemma 6.5.1.)

We present a description of fractional revival in matrix form.

9.9.4 Corollary. *If we have fractional* (α,β)*-revival on vertices* a *and* b *at time* τ*, the subspace spanned by* e_a *and* e_b *is* $U(\tau)$*-invariant; if* $\beta \neq 0$ *the matrix that represents the action of* $U(\tau)$ *on this subspace is*

$$\begin{pmatrix} \alpha & \beta \\ \beta & -\frac{\overline{\alpha}\beta}{\overline{\beta}} \end{pmatrix}. \qquad \square$$

You should convince yourself that the matrix R is unitary (its determinant is $\beta/\overline{\beta}$). Since it is unitary and not a scalar matrix, its eigenvalues are distinct. Note that this result shows that $U(\tau)$ is block-diagonal, with one block of order 2×2 and, if $n = |V(X)|$, the other block of order $(n-2)\times(n-2)$.

Since D_S is real, Theorem 9.1.1 tells us that the eigenvalue support of $\{a,b\}$ must satisfy the ratio condition. Recall that the eigenvalue support of D is the set of eigenvalue pairs (θ_r,θ_s) such that $E_rDE_r \neq 0$. You might show (see the Exercises) that if $E_rDE_s \neq 0$, then neither E_rDE_r nor E_sDE_s is zero.

9.10 Commutativity

We investigate the interaction of commutativity (of the induced algebra) and fractional revival.

9.10.1 Lemma. *If we have proper fractional revival on* $S = \{a,b\}$*, then* $\mathcal{A}(S)$ *is commutative.*

Proof. Assume $S = \{a,b\}$. If we have fractional (α,β)-revival at time τ and if we set $R(t) = (U(t)_{S,S})$. If $R(\tau)$ has only one eigenvalue then, since $R(\tau)$ is unitary, it must be a scalar multiple of I_2. Since our revival is proper $\beta \neq 0$ and so, by Corollary 9.9.4, the eigenvalues of $R(\tau)$ are distinct. From this we infer that any matrix that commutes with $R(\tau)$ is a polynomial in $R(\tau)$. $\square$

To help us make use of this lemma, we provide a characterization of commutativity for symmetric matrices.

9.10.2 Lemma. *If* $\beta \neq 0$*, the matrices*

$$\begin{pmatrix} \alpha & \beta \\ \beta & \gamma \end{pmatrix}, \quad \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

commute if and only if

$$\frac{a-c}{b} = \frac{\alpha-\gamma}{\beta}.$$

Proof. Two symmetric matrices commute if and only their product is symmetric. Denote the matrices in the statement of the lemma by A and B. If we compute the off-diagonal entries of AB, we see that AB is symmetric if and only if

$$\alpha b + \beta c = \beta a + \gamma c. \qquad \square$$

If $\beta = 0$ and $\alpha = \gamma$, then A is a scalar matrix and commutes with all 2×2 matrices; if $\beta = 0$ and $\alpha \neq \gamma$ then the matrices that commute with A are the polynomials in A, and are all diagonal.

(In some sense, the previous lemma still holds when $b = 0$.)

9.10.3 Corollary. *If we have proper fractional (α, β)-revival on $\{a, b\}$ at time τ and*

$$B = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

commutes with $(U(\tau))_{S,S}$, then

$$\frac{a-c}{b} = \left(\frac{\alpha}{\beta} + \frac{\overline{\alpha}}{\overline{\beta}}\right).$$

Proof. We recall that

$$(U(\tau))_{S,S} = \begin{pmatrix} \alpha & \beta \\ \beta & -\frac{\overline{\alpha}\beta}{\overline{\beta}} \end{pmatrix}$$

and apply the lemma. $\square$

There are a number of places where we can apply this corollary. If $S = \{a, b\}$ and we set

$$((tI - A)^{-1})_{S,S} = \begin{pmatrix} \phi(X \setminus t) & \phi_{a,b}(X, t) \\ \phi_{a,b}(X, t) & \phi(X \setminus b, t) \end{pmatrix},$$

then $((tI - A)^{-1})_{S,S}$ lies in $\mathcal{A}(S)$ and so it commutes with $(U(\tau))_{S,S}$. If $\mathcal{P}(a, b)$ denotes the set of paths from a to b in X, then (from Section 4.3)

$$\begin{aligned} \phi_{a,b}(X, t) &= \sum_{P \in \mathcal{P}(a,b)} \phi(X \setminus P, t) \\ &= (\phi(X \setminus a, t)\phi(X \setminus b, t) - \phi(X, t)\phi(X \setminus \{a, b\}, t))^{1/2}. \end{aligned}$$

9.10.4 Corollary. *If we have proper fractional* (α, β)*-revival on* $\{a, b\}$ *at time* τ*, then*

$$\phi(X \setminus a, t) - \phi(X \setminus b, t) = \left(\frac{\alpha}{\beta} + \frac{\overline{\alpha}}{\overline{\beta}}\right)\phi_{a,b}(X, t). \qquad \square$$

Note that if $\phi(X \setminus a, t) - \phi(X \setminus b, t)$ is a scalar times $\phi_{a,b}(X, t)$, then the scalar is determined by the leading coefficients of $\phi(X \setminus a, t) - \phi(X \setminus b, t)$ and $\varphi_{a,b}(t)$. Hence this corollary holds if $\phi(X \setminus a, t) - \phi(X \setminus b, t)$ is a scalar times $\phi_{a,b}(X, t)$. In fact:

9.10.5 Lemma. *If* $a, b \in V(X)$*, there is a constant* μ *such that*

$$\phi(X \setminus a, t) - \phi(X \setminus b, t) = \mu\phi_{a,b}(X, t),$$

if and only if the induced algebra on $\{a, b\}$ *is commutative.*

Proof. If the stated condition holds, then for all t, the matrices

$$\begin{pmatrix} \phi(X \setminus t) & \phi_{a,b}(X, t) \\ \phi_{a,b}(X, t) & \phi(X \setminus b, t) \end{pmatrix}$$

commute. But if $S = \{a, b\}$,

$$\begin{pmatrix} \phi(X \setminus a, t) & \phi_{a,b}(X, t) \\ \phi_{a,b}(X, t) & \phi(X \setminus b, t) \end{pmatrix} = ((tI - A)^{-1})_{S,S} = \sum_r \frac{1}{t - \theta_r}(E_r)_{S,S}$$

from which we deduce that the matrices $(E_r)_{S,S}$ commute. $\square$

If a and b are cospectral vertices, then $\phi(X \setminus a, t) = \phi(X \setminus b, t)$ and so the induced algebra is commutative. In this case all matrices in it have constant diagonal, and so they have the form

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}$$

and we can see, without appeal to the above machinery, that they commute.

9.10.6 Corollary. *If we have proper fractional* (α, β)*-revival on* $\{a, b\}$ *and* $a \sim b$*, then* a *and* b *are cospectral.*

Proof. If $a \sim b$, then $\mathcal{P}(a,b)$ contains unique path of length two, and so $\deg(\varphi_{a,b}) = n-2$. On the other hand both $\phi(X \setminus a, t)$ and $\phi(X \setminus b, t)$ are monic polynomials of degree $n-1$ and in both polynomials, the coefficient of t^{n-2} is zero (no loops). Hence the degree of $\phi(X \setminus a, t) - \phi(X \setminus b, t)$ is at most $n-3$. It follows that $\phi(X \setminus a, t) - \phi(X \setminus b, t)$ must be the zero polynomial. □

Other simple conditions that imply cospectrality are given in the Exercises.

We say two vertices a and b are *fractionally cospectral* if their induced algebra $\mathcal{A}(\{a,b\})$ is commutative. They are *strongly fractional cospectral* if they are fractionally cospectral and parallel.

We have *balanced* fractional (α,β)-revival on $\{a,b\}$ at time τ if $|\alpha| = |\beta|$.

9.10.7 Lemma. *If a and b are cospectral, then there is balanced fractional revival at time τ if and only if there is perfect state transfer at time 2τ.*

Proof. If a and b are cospectral, then $(U_S(t))_a = (U_S(t))_b$ (for all t). If we have pst at time 2τ, then

$$U_S(2\tau) = \gamma \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Now

$$\begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}^2 = \begin{pmatrix} \alpha^2 + be^2 & 2\alpha\beta \\ 2\alpha\beta & \alpha^2 + \beta^2 \end{pmatrix}$$

and so if $(U_S(2\tau))_{a,a} = 0$, then $\beta = \pm i\alpha$. So there is a complex scalar ζ of norm one such that

$$U_S(2\tau) = \zeta \begin{pmatrix} 1 & \pm i \\ \pm i & 1 \end{pmatrix}$$

and thus we have balanced fractional revival at time τ.

We leave the converse as an exercise. □

If we have balanced fractional revival on cospectral vertices at time τ, you may show that there is a complex scalar ζ of norm one such that

$$(U(\tau)_{S,S})^4 = \zeta I_2$$

and hence there is perfect state transfer from a to b at time 2τ.

If D_S is periodic at time t, then

$$D_S = U(t)D_SU(-t),$$

and

$$D_S = (D_SU(t)D_S)(D_SU(-t)D_S) = U(t)_{S,S}U(-t)_{S,S} = U(t)_{S,S}(U(t)_{S,S})^*.$$

It follows that if D_S is periodic at time τ, then $U(\tau)_{S,S}$ is unitary. (Note that $(D_S)_{S,S}$ is the identity matrix $I_{|S|}$.)

9.11 Cospectrality

We investigate fractional revival on cospectral vertices. If a and b are cospectral vertices and M is a polynomial in A, them $M_{a,a} = M_{b,b}$. Setting $S = \{a, b\}$, we conclude consists all matrices

$$\begin{pmatrix} \gamma & \sigma \\ \sigma & \gamma \end{pmatrix}, \qquad \gamma, \sigma \in \mathbb{R}.$$

It follows at once that if a and b are cospectral, the induced algebra on S is commutative. We see that

$$U(\tau) = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}$$

where $|\alpha|^2 + |\beta|^2 \leq 1$, and equality holds if and only if $U(t)$ is unitary (in which case we have fractional revival at time τ).

9.11.1 Theorem. *Assume a and b are cospectral vertices in X and that we have fractional revival on $S = \{a, b\}$. Then one of the following holds:*

(a) There is time τ at which both a and b are periodic.

(b) There is perfect state transfer from a to b.

(c) There is pretty good state transfer from a to b.

Proof. Assume that fractional revival takes place at time τ. Then

$$U(\tau) = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}$$

with $|\alpha|^2 + |\beta|^2 = 1$. In particular, $U(\tau)$ is unitary and this implies that

$$\alpha\overline{\beta} + \beta\overline{\alpha} = 0.$$

Consequently

$$\frac{\overline{\alpha}}{\overline{\beta}} = -\frac{\alpha}{\beta}$$

and therefore there is a complex number ζ of norm 1 and a real number θ such that

$$U(\tau) = \zeta \begin{pmatrix} \cos(\theta) & i\sin(\theta) \\ i\sin(\theta) & \cos(\theta) \end{pmatrix}.$$

As

$$\begin{pmatrix} \cos(\theta) & i\sin(\theta) \\ i\sin(\theta) & \cos(\theta) \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} -i & 0 \\ 0 & 1 \end{pmatrix},$$

we see that $\zeta^{-1}U(\tau)$ is conjugate to rotation by θ.

If the multiplicative order of $\zeta^{-1}U(\tau)$ is $2m+1$, then we have periodicity at a and b at time $(2m+1)\tau$.

If the multiplicative order of $\zeta^{-1}U(\tau)$ is $2m$, then

$$U(m\tau) = \zeta^m \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

and so we have perfect state transfer at time $m\tau$ (and simultaneous periodicity at time $2m\tau$).

If the multiplicative order of $\zeta^{-1}U(\tau)$ is infinite, θ is irrational. It follows that if $\epsilon > 0$, there an integer m such that $\zeta^{-1}U(m\tau)$ lies within ϵ of

$$\begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -i & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

Accordingly there is pretty good state transfer from a to b.

The results from the previous section show that, in many cases, fractional revival implies cospectrality. However that are graphs where there is fractional revival between non-cospectral vertices; we describe one example. Let S and T be the stars $K_{1,a+k}$ and $K_{1,b+k}$ (with $a, b \geq 1$ and $k \geq 2$) and let X the graph we get by identifying k vertices of degree one in S with k vertices of degree one in T. Then the two vertices of X of degree greater that two are fractionally cospectral and there are infinitely many triples (a, k, b) such that there is fractional revival on these vertices (the first of which is $(3, 2, 6)$).

9.12 Characterizing Fractional Revival

Assume $S = \{a, b\} \subseteq V(X)$ and $D = D_S$. Set $U_S(\tau) = (U(t)_{S,S})$ and $F_r = (E_r)_{S,S}$.

9.12.1 Lemma. *If S is parallel, the eigenvalue support of D_S is the set of pairs*

$$\{(\theta_r, \theta_s) : F_r F_s \neq 0\}.$$

Proof. As defined, the eigenvalue support consists of the pairs (θ_r, θ_s) such that $E_r D E_s \neq 0$. We note that

$$\langle E_r D E_s, E_r D E_s\rangle = \operatorname{tr} E_s D E_r E_r D E_s = \operatorname{tr} E_s D E_r D E_s$$

and, as $D = D^2$,

$$\operatorname{tr} E_s D E_r D E_s = \operatorname{tr} D E_s D E_r D = \operatorname{tr} D E_s D\, D E_r D = \operatorname{tr} F_s F_r.$$

Since F_r and F_s are positive semidefinite, $\operatorname{tr}(F_r F_s) = 0$ if and only if $F_r F_s = 0$. □

It is worth noting that if M and N are rank-one matrices, then $MN = NM$ if and only if $MN = 0$ or $N = cM$ for some scalar c.

9.12.2 Theorem. *Let a and b be distinct vertices of the connected graph X. We have fractional revival on $S = \{a, b\}$ at time τ if and only if the following hold:*

(a) a and b are parallel.

(b) The induced adjacency algebra on S is commutative.

(c) Let C^+ be set of indices r such $(E_r)_{a,b} > 0$, and let C^- be set of indices r such $(E_r)_{a,b} < 0$. Then the square of the difference of two eigenvalues from C^+ or C^- is an integer, and all these integers have the same square-free part.

Proof. We show that the stated conditions are necessary, and leave their sufficiency as an exercise.

We have fractional revival on S if and only if D_S is periodic, and therefore the conclusions in part (c) are consequences of Theorem 9.5.1.

We first treat the case where U_S is diagonal. If $U(t) = \gamma I$, and we have simultaneous periodicity on a and b, which counts as fractional revival. If $U_S(\tau)$ is diagonal but not a scalar, then any matrix that commutes with $U_S(\tau)$ is diagonal. This implies that $(E_r)_{a,b} = 0$ for all r and therefore

$$(A^k)_{a,b} = \sum_r \theta_r^k (E_r)_{a,b} = 0$$

for all k. This implies that a and b lie in different components of X, contradicting our assumption that X is connected.

We assume now that $U_S(\tau)$ is not diagonal, and that its eigenvalues are distinct. Since S is parallel, $\mathrm{rk}(F_r) \leq 1$ for all r. If

$$F_r = xx^T, \quad F_s = yy^T$$

then

$$F_r F_s = (x^T y) x y^T$$

and it follows that F_r and F_s commute if and only if x and y are parallel or orthogonal; equivalently either $F_r F_s = 0$ or F_s is a nonzero scalar multiple of F_r. If

$$x = \begin{pmatrix} w \\ z \end{pmatrix}$$

and $x^T y = 0$, then y must be a scalar multiple of

$$\begin{pmatrix} -z \\ w \end{pmatrix}.$$

Therefore F_r is a scalar multiple of one the matrices

$$\begin{pmatrix} w^2 & wz \\ wz & z^2 \end{pmatrix}, \qquad \begin{pmatrix} z^2 & -wz \\ -wz & w^2 \end{pmatrix}.$$

Note that one of these matrices has all entries non-negative while, in the other, only the off-diagonal entries are negative.

The matrix $U_S(\tau)$ is normal, so has a spectral decomposition with idempotents Φ and $I - \Phi$, where we may assume that the entries of Φ are non-negative. For each r, one of the following holds:

$$F_r = \mathrm{tr}(F_r)\Phi, \quad F_r = \mathrm{tr}(F_r)(I - \Phi)$$

Choose indices r in C^+ and s in C^- and set $\theta^+ = \theta_r$ and $\theta^- = \theta_s$. If $r \in C^+$ we have $U_S(\tau)F_r = e^{i\tau\theta^+}F_r$ and if $r \in C^-$ we have $U_S(\tau)F_r = e^{i\tau\theta^-}F_r$.

We note that if r, s both lie in C^+ or in C^- if and only if $F_rF_s \neq 0$, implying that C^+ and C^- are closed under taking algebraic conjugates. We can paraphrase Theorem 7.6.1 as stating that if the ratio condition holds for a set Φ of eigenvalues, closed under algebraic conjugates, then the squared difference of any two eigenvalues from Φ is an integer and the square-free part of each squared difference is the same. Because $e^{i\tau\theta_r}$ is constant on C^+ and C^-, it follows that the ratio condition holds for the sets

$$\{\theta_r : r \in C^+\}, \quad \{\theta_s : s \in C^-\}.$$

Therefore there is a square-free integer Δ and integers $m_{r,s}$ such that for each $r, s \in C^+$, or $r, s \in C^-$, we have

$$\theta_r - \theta_s = m_{r,s}\sqrt{\Delta}.$$

If g is the gcd of the integers $m_{r,s}$, then

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

We see that

$$\begin{aligned} U_S(\tau) &= \sum_{r\in C+} e^{i\tau\theta_r}F_r + \sum_{r\in C^-} e^{i\tau\theta_r}F_r \\ &= \theta^+\left(\sum_{r\in C^+}\operatorname{tr}(F_r)\right)\Phi + \theta^-\left(\sum_{r\in C^-}\operatorname{tr}(F_r)\right)(I-\Phi) \end{aligned}$$

This is a version of the spectral decomposition of $U_S(\tau)$. Since $U_S(\tau)$ is normal, it is unitary if and only if its eigenvalues have norm one, and it is unitary if and only D_S is periodic at time τ, i.e., if only there is fractional revival at time τ. As $\sum_r F_r = I_2$, we have $\sum_r \operatorname{tr}(F_r) = 2$ and therefore the eigenvalues of $U_S(\tau)$ have norm one if and only if

$$\sum_{r\in C^+}\operatorname{tr}(F_r) = 1. \tag{9.12.1}$$

(In which case, $\sum_{r\in C^+} F_r = \Phi$.) Now

$$I_2 = \sum_r F_r = \left(\sum_{r\in C^+}\operatorname{tr}(F_r)\right)\Phi + \left(\sum_{r\in C^-}\operatorname{tr}(F_r)\right)(I-\Phi).$$

and, since both eigenvalues of I_2 are equal to 1 we deduce that (9.12.1) holds. □

Notes

Exercises

9-1. Prove that if the induced algebra on $\{a, b\}$ is commutative, there is a constant μ such that

$$(E_r)_{a,a} - (E_r)_{b,b} = \mu (E_r)_{a,b}.$$

Deduce that if X is regular and connected, the vertices a and b are cospectral.

9-2. Prove that if we have proper fractional revival on $\{a, b\}$ and either of the following conditions hold, then a and b are cospectral:

(a) X is bipartite and $\operatorname{dist}(a, b)$ is odd.

(b) a and b have the same valency and $\operatorname{dist}(a, b) = 2$.

9-3. Assume S is a periodic subset of $V(X)$, with period τ. Show that if the eigenvalues of $(U(\tau)_{S,S})$ are simple, the induced algebra at S is commutative with dimension at most $|S|$.

9-4. Prove that if $E_r D_S E_r = 0$, then $E_r D_S E_s = 0$ for all s.

9-5. Assume $S = \{1, 2\}$ and

$$A = \begin{pmatrix} A_0 & B \\ B^T & A_1 \end{pmatrix}, \qquad U(\tau) = \begin{pmatrix} U_0 & 0 \\ 0 & U_1 \end{pmatrix}.$$

(So we have fractional revival on S at time τ and $U_0 = (U(\tau)_{S,S})$.) Show that U_0 commutes with BB^T.

9-6. Assume we have fractional revival on $\{a, b\}$ at time τ. Show that if $\deg(a) \neq \deg(b)$ and a and b have no common neighbour, then a and b are simultaneously periodic at time τ.

Chapter 10

Paths and Trees

We investigate the spectral properties of paths, and show that there is no perfect state transfer on paths with more than three vertices. We present the proof, due to Coutinho and Liu, that perfect state transfer relative to the Laplacian does not occur on any tree with more than two vertices.

10.1 Recurrences for Paths

Let P_n denote the path on n vertices and let $\phi_n(t)$ denote its characteristic polynomial. Then it's simple enough to verify that

$$\phi_0(t) = 1, \quad \phi_1(t) = t, \quad \phi_2(t) = t^2 - 1, \quad \phi_3(t) = t^3 - 2t.$$

(For example, use the fact that paths are bipartite and that the coefficient of x^{n-2} in the characteristic polynomial of a graph on n vertices is the number of edges.) To go further we note that

$$\det \begin{pmatrix} a & b^T \\ b & A_1 \end{pmatrix} = \det \begin{pmatrix} a & 0 \\ b & A_1 \end{pmatrix} + \det \begin{pmatrix} 0 & b^T \\ b & A_1 \end{pmatrix}$$

and hence

$$\begin{aligned} &\det \begin{pmatrix} t & -e_1^T \\ -e_1 & tI - A(P_n) \end{pmatrix} \\ &\quad = \det \begin{pmatrix} t & 0 \\ -e_1 & tI - A(P_n) \end{pmatrix} + \det \begin{pmatrix} 0 & -e_1^T \\ -e_1 & tI - A(P_n) \end{pmatrix} \\ &\quad = \det \begin{pmatrix} t & 0 \\ -e_1 & tI - A(P_n) \end{pmatrix} - \det(tI - A(P_{n-1})). \end{aligned}$$

This leads to the basic recurrence:

10.1.1 Theorem.

$$\phi(P_{n+1}(t)) = t\phi(P_n, t) - \phi(P_{n-1}, t) \quad (n \geq 1). \qquad \square$$

Using this we can prove by induction that

$$\phi_n(t) = \sum_{k \geq 0} (-1)^k \binom{n-k}{k} t^{n-2k}.$$

We list the characteristic polynomials of the first six paths.

n	ϕ
1	t
2	$t^2 - 1$
3	$t^3 - 2t$
4	$t^4 - 3t^2 + 1$
5	$t^5 - 4t^3 + 3t$
6	$t^6 - 5t^4 + 6t^2 - 1$

If G and H are graphs then their 1-sum is the graph we get by identifying a vertex in G with a vertex in H. The resulting graph will depend on our choice of vertex and there is no harm in calling both vertices u (say). If Y is the 1-sum of G and H at the vertex u, then by Lemma 4.7.1

$$\phi(Y) = \phi(G \setminus u)\phi(H) + \phi(G)\phi(H \setminus u) - t\phi(G \setminus u)\phi(H \setminus u).$$

If X is obtained by joining a vertex u in G to a vertex v in H by an edge, then

$$\phi(X) = \phi(G)\phi(H) - \phi(G \setminus u)\phi(H \setminus v).$$

It is easy to derive this identity from the previous one, and it is also easy to use it to prove Theorem 10.1.1. You should also use it to prove the following generalization.

10.1.2 Lemma. *We have*

$$\phi_{m+n}(t) = \phi_m(t)\phi_n(t) - \phi_{m-1}(t)\phi_{n-1}(t).$$

We note some further interesting identities which we will not be using, the first is related to a property of the Fibonacci numbers:

$$\phi_n(t)^2 - \phi_{n-1}(t)\phi_{n+1}(t) = 1.$$

The second is an instance of a *Christoffel-Darboux identity*, which hold for orthogonal polynomials in general and not just for characteristic polynomials of paths:

$$\sum_{r=0}^{n-1} \phi_r(s)\phi_r(t) = \frac{\phi_{n-1}(s)\phi_n(t) - \phi_n(s)\phi_{n-1}(t)}{t-s}$$

This is easily verified by induction and implies that

$$\sum_{r=0}^{n-1} \phi_r(t)^2 = \phi_{n-1}(t)\phi_n'(t) - \phi_{n-1}'(t)\phi_n(t).$$

10.2 Eigenvalues and Eigenvectors

We write our recurrences in matrix form:

$$\begin{pmatrix}\phi_{n+1}\\ \phi_n\end{pmatrix} = \begin{pmatrix} t & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_n\\ \phi_{n-1}\end{pmatrix}$$

$$\begin{pmatrix}\phi_{n+1}\\ \phi_n\end{pmatrix} = \begin{pmatrix} t & -1\\ 1 & 0\end{pmatrix}^n\begin{pmatrix}t\\ 1\end{pmatrix}$$

and then convert to generating functions:

$$\begin{aligned}\sum_{n\geq 0} u^n \begin{pmatrix}\phi_{n+1}\\ \phi_n\end{pmatrix} &= \left(I - u\begin{pmatrix} t & -1\\ 1 & 0\end{pmatrix}\right)^{-1}\begin{pmatrix}t\\ 1\end{pmatrix}\\ &= \begin{pmatrix} 1-ut & u\\ -u & 1\end{pmatrix}^{-1}\begin{pmatrix}t\\ 1\end{pmatrix}\\ &= \frac{1}{1-ut+u^2}\begin{pmatrix} 1 & -u\\ u & 1-ut\end{pmatrix}\begin{pmatrix}t\\ 1\end{pmatrix}\\ &= \frac{1}{1-ut+u^2}\begin{pmatrix} t-u\\ 1\end{pmatrix}\end{aligned}$$

10.2.1 Lemma.
$$\sum_{n\geq 0} u^n \phi_n = \frac{1}{1-ut+u^2}$$

If
$$\alpha = \frac{1}{2}(t+\sqrt{t^2-4}), \quad \beta = \frac{1}{2}(t-\sqrt{t^2-4})$$
then
$$\begin{aligned}\frac{1}{1-ut+u^2} &= \frac{1}{(1-\alpha u)(1-\beta u)}\\ &= \frac{1}{\alpha-\beta}\left(\frac{\alpha}{1-\alpha u}-\frac{\beta}{1-\beta u}\right)\end{aligned}$$
and
$$\phi_n = \frac{\alpha^{n+1}-\beta^{n+1}}{\alpha-\beta}.$$

Now put $t = 2\cos(\zeta)$. Then
$$\alpha = \cos(\zeta)+i\sin(\zeta) = e^{i\zeta}, \qquad \beta = \cos(\zeta)-i\sin(\zeta) = e^{-i\zeta}$$
and
$$\phi_n(2\cos(\zeta)) = \frac{e^{(n+1)i\zeta}-e^{-(n+1)i\zeta}}{e^{i\zeta}-e^{-i\zeta}}.$$

10.2.2 Theorem.
$$\phi_n(2\cos(\zeta)) = \frac{\sin(n+1)\zeta}{\sin(\zeta)}.$$
□

10.2.3 Corollary. *The eigenvalues of* P_n *are*
$$2\cos\left(\frac{\pi k}{n+1}\right), \quad k = 1,\dots,n.$$
□

Once we have the eigenvalues, the eigenvectors are easy. If $A = A(P_n)$ then
$$(tI-A)\begin{pmatrix}\phi_0(t)\\ \vdots\\ \phi_{n-1}(t)\end{pmatrix} = \phi_n(t)e_n,$$

where e_n is the last vector in the standard basis. Hence if θ_j is the j-th eigenvalue of P_n, then the corresponding eigenvector is

$$z_j = \begin{pmatrix} \phi_0(\theta_j) \\ \vdots \\ \phi_{n-1}(\theta_j) \end{pmatrix}$$

We could use the Christoffel-Darboux identity to deduce that

$$\sum_{r=0}^{n-1} \phi_r(\theta_j)^2 = -\phi_{n-1}(\theta_j)\phi_n'(\theta_j),$$

but instead we will use the following:

10.2.4 Lemma.

$$2\sum_{r=0}^{n} \cos(r\theta) = \frac{\sin((n+\frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} + 1.$$

Proof. If $q := e^{i\theta}$ then

$$\begin{aligned}
2\sum_{r=0}^{n} \cos(r\theta) = \sum_{r=0}^{n}(e^{ir\theta} + e^{-ir\theta}) &= \sum_{r=0}^{n}(q^r + q^{-r}) \\
&= \frac{q^{n+1}-1}{q-1} + \frac{q^{-n-1}-1}{q^{-1}-1} \\
&= \frac{q^{n+1}-q^{-n}}{q-1} + 1 \\
&= \frac{q^{n+1/2}-q^{-1/2-n}}{q^{1/2}-q^{-1/2}} + 1 \\
&= \frac{\sin((n+\frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} + 1.
\end{aligned}$$

□

Using Theorem 10.2.2, we have

$$\sum_{r=0}^{n-1} \phi_r(2\cos(u))^2 = \frac{1}{\sin^2(u)} \sum_{r=0}^{n-1} \sin^2(ru)$$

and

$$\begin{aligned}
\sum_{r=0}^{n} \sin^2(ru) &= \sum_{r=0}^{n} \frac{1}{2}(1-\cos(2ru)) \\
&= \frac{n+1}{2} - \frac{1}{4}\left(\frac{\sin((2n+1)u)}{\sin(u)} + 1\right).
\end{aligned}$$

Now set $u = j\pi/(n+1)$. Then $(2n+1)u = 2j\pi - u$ and

$$\frac{\sin((2n+1)u)}{\sin(u)} = \frac{\sin(2j\pi - u)}{\sin(u)} = -1$$

whence

$$\sum_{r=0}^{n-1} \phi_r(2\cos(u))^2 = \frac{n+1}{2\sin(u)}.$$

10.2.5 Lemma. *The idempotents $E_1, \dots, E_n$ in the spectral decomposition of P_n are given by*

$$(E_r)_{j,k} = \frac{2}{n+1} \sin\left(\frac{jr\pi}{n+1}\right) \sin\left(\frac{kr\pi}{n+1}\right).$$

Proof. If $A = A(P_n)$ and e_n is the n-th vector in the standard basis of $\mathbb{R}^n$, then

$$A \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix} = \begin{pmatrix} \sin(2\beta) \\ \sin(\beta) + \sin(3\beta) \\ \vdots \\ \sin((n-1)\beta) \end{pmatrix} = 2\cos(\beta) \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix} - \sin((n+1)\beta) e_n$$

So if $\sin((n+1)\beta) = 0$ then

$$z(\beta) := \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix}$$

is an eigenvector for A with eigenvalue $2\cos(\beta)$. Letting β vary over the values

$$\frac{2\pi r}{n+1}, \quad r = 1, \dots, n$$

we obtain n distinct eigenvalues. Therefore each eigenvalue of P_n is simple and the projection onto the eigenspace spanned by $z(\beta)$ is

$$\frac{1}{z(\beta)^T z(\beta)} z(\beta) z(\beta)^T).$$

We can compute the value of the inner product $z(\beta)^T z(\beta)$ using 10.2.4, and this yields the stated expression for E_r. □

10.2.6 Lemma. *The polynomials ϕ_n and ϕ_{n-1} are coprime.*

Proof. Since

$$\phi_{m+1}(t) = t\phi_m(t) - \phi_{m-1}(t)$$

we see that any common factor of ϕ_{m+1} and ϕ_m must divide ϕ_{m-r} for $r = 0, 1, \ldots, m$. □

10.2.7 Corollary. *If θ is a zero of $\phi_n(t)$ then no two consecutive entries of the corresponding eigenvector are zero, and the first and last entries are not zero.*

10.2.8 Theorem. *If*

$$\theta_j = 2\cos\left(\frac{\pi j}{n+1}\right)$$

then

$$\phi_{m-1}(\theta_j) = \frac{\phi_{mj-1}(\theta_1)}{\phi_{j-1}(\theta_1)}$$

It is very easy to derive this from the sine-formula for ϕ_n. Hence we obtain

$$\phi_r(\theta_2) = \frac{\phi_{2r+1}(\theta_1)}{\phi_1(\theta_1)};$$

if $2r+1 > n$ then

$$\phi_{2r+1} = \phi_n\phi_{2r+1-n} - \phi_{n-1}\phi_{2r-n}$$

and therefore

$$\phi_{2r+1}(\theta_1) = -\phi_{n-1}(\theta_1)\phi_{2r-n}(\theta_1) = -\phi_{2r-n}(\theta_1).$$

10.3 Line Graphs and Laplacians

10.3.1 Theorem. *If X is bipartite on $m+n$ vertices with color classes $\{1, \ldots, m\}$ and $\{m+1, \ldots, m+n\}$, then*

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

If D is the diagonal matrix of order $(m+n) \times (m+n)$ with $D_{i,i} = 1$ when $i \le m$ and $D_{i,i} = -1$ otherwise, $DAD = -A$.

Since $D^2 = I$, if $DAD = -A$ then A and $-A$ are similar. This implies that the spectrum of X is symmetric about 0. Further if $Az = \theta z$ then

$$ADz = D(DAD)z = -DAz = -\theta Dz$$

and so D pairs the eigenvectors of A.

Let Δ denote the diagonal matrix of valencies of X. Then $\Delta - A$ is the *Laplacian matrix* of X. If X is bipartite and D is as before, then

$$DLD = \Delta - DAD = \Delta + A.$$

The matrix $\Delta + A$ is known as the *unsigned Laplacian*.

If B is the vertex-edge incidence matrix of X, then

$$BB^T = A(X) + \Delta$$

and

$$B^T B = A(L(X)) + 2I$$

Therefore $A(X) + \Delta$ and $A(L(X)) + 2I$ have the same nonzero eigenvalues with the same multiplicities.

10.3.2 Corollary. *If X is bipartite then $A(L(X)) + 2I$ and $\Delta - A(X)$ have the same non-zero eigenvalues with the same multiplicities.* □

For the path P_n we have

$$L(P_n) = P_{n-1}.$$

10.3.3 Corollary. *$A(P_{n-1}) + 2I$ and $\Delta - A(P_n)$ have the same nonzero eigenvalues with the same multiplicities.* □

If $BB^T z = \lambda z$ then

$$(B^T B)B^T z = B^T BB^T z = \lambda B^T z$$

Thus if z is an eigenvector for BB^T with eigenvalue λ and $\lambda \neq 0$, then $B^T z$ is an eigenvalue for $B^T B$ with eigenvalue λ.

Similarly if $B^T By = \lambda y$ then

$$(BB^T)By = BB^T By = \lambda By$$

and so if $\lambda \neq 0$ we see that By is an eigenvector for BB^T with eigenvalue λ.

Suppose θ is an eigenvalue of P_{n-1} and B is the vertex-edge incidence matrix of P_n. Then

$$B^T B = 2I + A(P_{n-1}), \qquad BB^T = \Delta + A(P_n)$$

and so if θ is an eigenvalue of $A(P_{n-1})$ then $\theta+2$ is an eigenvalue of $\Delta+A(P_n)$. We know that Z_{n-1} is the eigenvector of P_{n-1} with eigenvalue θ, and so Bz is an eigenvector of $\Delta + A(P_n)$ with eigenvalue $\theta + 2$. By changing the sign of the entries indexed by a color class, we obtain an eigenvector for $\Delta - A(P_n)$ with the same eigenvalue.

Since

$$\cos\left(\frac{(n-r)\pi}{n}\right) = -\cos\left(\frac{r\pi}{n}\right),$$

for Laplacian eigenvalues of P_n we have

$$\theta_r + \theta_{n-r} = 4.$$

10.4 Inverses

If n is even, $A(P_n)$ is invertible. If we order the odd vertices before the even vertices then

$$A(P_n) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

where if $n = 8$ we have

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

If $N := B - I$, then $N^4 = 0$ and so in general

$$B^{-1} = (I + N)^{-1} = \sum_{k=0}^{n-1} (-1)^k N^k.$$

Note that A is invertible if and only if B is:

$$A^{-1} = \begin{pmatrix} 0 & B^{-T} \\ B^{-1} & 0 \end{pmatrix}.$$

If $n = 8$, this yields

$$B^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 \end{pmatrix}$$

and if

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

then

$$DB^{-1}D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

If we denote this matrix by C then we see that

$$\begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} 0 & B^{-T} \\ B^{-1} & 0 \end{pmatrix} \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} = \begin{pmatrix} 0 & C^T \\ C & 0 \end{pmatrix}$$

and the last matrix is the adjacency matrix of a graph with P_8 as a subgraph.

10.5 Eigenthings for Laplacians of Paths

Let Δ denote the diagonal matrix with i-th diagonal entry equal to the valency of the i-th vertex of X. Then the Laplacian of X is $\Delta - A$. Let B be the $n \times (n-1)$ matrix with

$$B_{i,i} = 1, \quad B_{i,i-1} = -1$$

and all other entries zero. Then B is the incidence matrix of an orientation of P_n and

$$BB^T = \Delta - A(P_n), \qquad B^T B = 2I - A(P_{n-1}).$$

We can also determine the idempotents in the spectral decomposition of $\Delta - A(P_n)$.

10.5.1 Lemma. *If $E_1, \dots, E_{n-1}$ are the idempotents in the spectral decomposition of P_{n-1}, then the idempotents of $\Delta - A(P_n)$ are $n^{-1}J$ and*

$$\frac{1}{2-\theta_r} BE_rB^T, \dots, r = 1, \dots, n-1.$$

Proof. Since

$$BE_rB^TBE_sB^T = BE_r(2I - A(P_{n-1})E_sB^T)$$

and since $E_rE_s = 0$ if $r \neq s$ and $(2I - A(P_{n-1})E_s = (2-\theta_s)E_s$, it follows that

$$BE_rB^TBE_sB^T = \delta_{r,s}(2-\theta_r)BE_rB^T.$$

Therefore $(2-\theta_r)^{-1}BE_rB^T$ is an idempotent. Next

$$(\Delta - A(P_n))BE_rB^T = BB^TBE_rB^T = B(2I - A(P_{n-1}))E_rB^T = (2-\theta_r)BE_rB^T$$

and therefore $(2-\theta_r)^{-1}BE_rB^T$ represents orthogonal projection onto an eigenspace of $A(P_n)$. The lemma follows. □

10.5.2 Lemma. *If $E_1, \dots, E_{n-1}$ are the idempotents in the spectral decomposition of P_{n-1}, and $1 \le j, k \le n$, then*

$$(2-\theta_r)^{-1}(BE_rB^T)_{j,k} = \frac{2}{n}\cos\left(\frac{(2j-1)r\pi}{2n}\right)\cos\left(\frac{(2k-1)r\pi}{2n}\right).$$

Proof. From 10.2.5, we have

$$(E_r)_{j,k} = \frac{2}{n}\sin\left(\frac{jr\pi}{n}\right)\sin\left(\frac{kr\pi}{n}\right), \qquad 1 \le j, k \le n-1.$$

Let $\alpha = r\pi/n$ and let σ denote the column vector of length $n-1$ where $\sigma_j = \sin(j\alpha)$. Then

$$BE_rB^T = \frac{2}{n}B\sigma(B\sigma)^T$$

and

$$B\sigma = \begin{pmatrix} \sin(\alpha) \\ \sin(2\alpha) - \sin(\alpha) \\ \vdots \\ \sin((n-1)\alpha) - \sin((n-2)\alpha) \\ -\sin((n-1)\alpha) \end{pmatrix} = 2\sin(\alpha/2)\begin{pmatrix} \cos(\alpha/2) \\ \cos(3\alpha/2) \\ \vdots \\ \cos((2n-3)\alpha/2) \\ \cos((2n-1)\alpha/2) \end{pmatrix},$$

where in computing the last entry we have used the fact that $n\alpha = r\pi$, whence $\sin(n\alpha) = 0$ and

$$-\sin(n-1)\alpha = \sin(n\alpha) - \sin(n-1)\alpha.$$

Finally for P_{n-1} we have

$$2 - \theta_r = 2 - 2\cos\left(\frac{r\pi}{n}\right) = 4\sin^2\left(\frac{r\pi}{2n}\right)$$

10.6 No Transfer on Paths

In [20] Christandl et al. proved that perfect state transfer between the end-vertices of a path on n vertices did not occur if $n \geq 4$. We use our results on periodicity to show that perfect state transfer does not occur on any path on four or more vertices.

10.6.1 Theorem. *If $n \geq 4$, perfect state transfer does not occur on P_n.*

Proof. Suppose we have ab-pst on P_n, where $n \geq 4$, and let S denote the eigenvalue support of a. The spectrum of P_n lies in the open interval $(-2, 2)$ and, by Corollary **??** any two distinct eigenvalues in S differ by at least 1. It follows $|S| \leq 4$ and consequently the covering radius of a is at most three. An immediate consequence of this is that $n \leq 7$.

If $n = 7$ then the central vertex cannot be involved in pst, but the covering radius of any non-central vertex is at least four. If $n = 6$, the vertices with covering radius three are 3 and 4 and if $U(t)e_3 = \gamma e_4$, then

$$\gamma(e_3 + e_5) = \gamma A e_4 = AU(t)e_3 = U(t)Ae_3 = U(t)(e_2 + e_4);$$

Thus we also have pst from 2 to 5, but these vertices have covering radius four and therefore they cannot be involved in pst. We can rule out pst on P_5 by a similar process. For P_4 we also find that if we have pst between the central vertices, we have it between the end-vertices, and we have already ruled out this possibility. □

10.7 PST on Laplacians

In some respects, analysing perfect state transfer relative to the Laplacian is easier than that relative to the usual adjacency matrix:

10.7.1 Lemma. *If $U(t)$ is the transition matrix relative to the Laplacian of a graph and perfect state transfer from a to b occurs, then $U(t)e_a = e_b$.*

Proof. Since $(\Delta - A)\mathbf{1} = 0$, it follows that $U(t)\mathbf{1} = \mathbf{1}$. If $U(t)e_a = \gamma e_b$, then

$$\gamma = \gamma \mathbf{1}^T e_b = \mathbf{1}^T U(t) e_a = \mathbf{1}^T e_a = 1. \qquad \square$$

If L is the Laplacian of P_2, then $L = I - A$ and

$$U(t) = \exp(it(I - A)) = e^{it} \exp(-itA).$$

It follows that we have perfect state transfer on P_2 when we use the Laplacian.

We need to work with strongly cospectral vertices relative to the Laplacian. The proofs we gave for strongly cospectral vertices relative to the adjacency matrix go through without change but, since such claims are often risky, we briefly derive what we are about to use.

Assume L has the spectral decomposition

$$L = \sum_{r=1}^{m} \lambda_r F_r$$

where $\lambda_1 = 0$ and $\lambda_1 \le \cdots \le \lambda_m$ and suppose $U(t) = \exp(itL)$. If we have ab-pst then $U(t)e_a = e_b$ at some time t and so

$$F_r e_b = F_r U(t) e_a = e^{it\lambda_r} F_r e_a;$$

since Fe_r and Fe_b are real, this implies that $e^{it\lambda_r} = \pm 1$. We also see that

$$e_b^T F_r e_b = e_a^T F_r e_a$$

and thus if we have Laplacian pst from a and b, then a and b are strongly cospectral. As with the adjacency matrix, cospectral vertices have the same eigenvalue support.

If a and b are strongly cospectral, then

$$(F_r)_{a,b} = e^{it\lambda_r} (F_r)_{a,a} = \pm (F_r)_{a,a}.$$

We will refer to the value of $e^{it\lambda_r}$ as the *sign* of λ_r relative to b. Equivalently it is the sign of $(F_r)_{a,b}$, for the eigenvalues λ_r in the eigenvalue support of a. If S is the eigenvalue support of a, we define S^+ and S^- to be the elements of S whose sign, relative to b, is respectively positive or negative. We recall that, by Lemma **??**, if X is periodic at a relative to the Laplacian, the eigenvalue support of a consists of integers. Hence we have the following characterisation of S^+.

10.7.2 Lemma. *Suppose we have perfect state transfer between vertices a and b in X relative to the Laplacian. Let S be the eigenvalue support of a and let g be the gcd of the elements of S. If $\lambda \in S$, then $\lambda \in S^+$ if and only if λ/g is even.* □

10.8 Twins

We define two vertices a and b to be *twins* if either $N(a) = N(b)$ or $a \cup N(a) = b \cup N(b)$. Our next result comes from Coutinho and Liu [24].

10.8.1 Lemma. *Suppose a and b are vertices in the connected graph X that are strongly cospectral, relative to the Laplacian. Then $|S^+| \geq 1$ and $|S^-| \geq 1$. If $|S^+| = 1$, then $|V(X)| = 2$; if $|S^-| = 1$, then a and b are twins.*

Proof. Define

$$z^+ = \sum_{S^+} F_r e_a, \qquad z^- = \sum_{S^-} F_r e_a.$$

Then $z^+ + z^- = e_a$ and $z^+ - z^- = e_b$, whence

$$z^+ = \frac{1}{2}(e_a + e_b), \qquad z^- = \frac{1}{2}(e_a - e_b).$$

The vector $\mathbf{1}$ is an eigenvector for L with eigenvalue zero. Hence $0 \in S^+$. If $|S^+| = 1$, then $e_a + e_b$ must be an eigenvector for L; since X is connected this implies that $|V(X)| = 2$.

Since $z^- \neq 0$ we see that $|S^-| \geq 1$ and, if equality holds then $e_a - e_b$ is an eigenvector for L. Let δ be the common valency of a and b. If $a \sim b$, then

$$L(e_a - e_b) = (\delta + 1)(e_a - e_b).$$

If $a \not\sim b$ then

$$L(e_a - e_b) = \delta(e_a - e_b).$$

In either case it follows that a and b are twins. □

The machinery at hand allows us to rule out perfect state transfer relative to the Laplacian on a large class of graphs. (This result is Lemma 4.2 from [24].)

10.8.2 Lemma. *If X is a graph with an odd number of vertices and an odd number of spanning trees, then Laplacian perfect state transfer does not occur on X.*

Proof. Assume $|V(X)| = n$. Suppose have pst from a to b and let S be the eigenvalue support of a. Since $0 \in S^+$, all elements of S^+ must be even. As is well known, n times the number of spanning trees in X is equal to the product of the non-zero eigenvalues of the Laplacian of X. This implies that $S^+ = \{0\}$, and hence that $n = 2$. □

10.9 No Laplacian Perfect State Transfer on Trees

The results in this section all come from Coutinho and Liu [24] `http://arxiv.org/abs/1408.2935`. Our first theorem implies that if we have Laplacian pst on a tree, then the vertices involved are twins (and therefore they have valency one).

Recall from Lemma **??** that if X is periodic at a vertex relative to the Laplacian, then the eigenvalue support consists of integers.

10.9.1 Theorem. *Let X be a connected graph and assume that the number of spanning trees in X is a power of two. If there is Laplacian perfect state transfer from a to b in X and S is the eigenvalue support of a, then $|S^-| = 1$.*

Proof. Suppose $\lambda \in S^-$, and assume that p is an odd prime that divides λ. As λ is an integer we may assume there is an integer eigenvector y with eigenvalue λ such that the gcd of the entries of y is 1.

We have $Ly = 0$ modulo p. As the number of spanning trees of X is a power of two, the kernel of L over $GF(p)$ has dimension one, and is spanned by $\mathbf{1}$, hence $y = k\mathbf{1}$ (modulo p), for some integer k. Since $\lambda \in S^-$ it follows that $y_a = -y_b$ and therefore, modulo p,

$$y_a + y_b = 2k.$$

As p is odd, this implies $k = 0$ modulo p, and this contradicts our choice of y. We conclude that the elements of S^- are powers of two, and now Lemma 10.7.2 implies that $|S^-| = 1$. □

10.9.2 Theorem. *If T is a tree with more than two vertices, then we cannot have perfect state transfer on T relative to the Laplacian.*

Proof. Assume that we have Laplacian pst from a to b in T. Then a and b are twins, whence they have valency one, and there is a unique vertex (c say) adjacent to a and b. The vector $e_a - e_b$ is therefore an eigenvector for $L(T)$ with eigenvalue 1. (And so $1 \in S^-$.) We can extend $e_a - e_b$ to an orthogonal basis for $\mathbb{R}^{V(X)}$, and we can assume that the new vectors in this basis are orthogonal to $e_a - e_b$.

By Lemma 10.8.1
$$\sum_{S^+} F_r e_a = \frac{1}{2}(e_a + e_b)$$
and therefore
$$\sum_{S^+} e_a^T F_r e_a = \frac{1}{2}$$
and
$$\sum_{S^+} e_c^T F_r e_a = 0. \tag{10.9.1}$$
We note now that $Le_a = e_a - e_c$ and so $e_c = (I - L)e_a$. Hence if $\lambda_r \in S^+$, then
$$e_c^T F_r e_a = e_a^T (I - L) F_r e_a = (1 - \lambda_r) e_a^T F_r e_a.$$
Therefore
$$\sum_{S^+} e_c^T F_r e_a = \sum_{S^+} (1 - \lambda_r) e_a^T F_r e_a.$$
Since each element of $S^+ \setminus 1$ is at least two,
$$\sum_{S^+} (1 - \lambda_r) e_a^T F_r e_a \le -\sum_{S^+} e_a^T F_r e_a = -\frac{1}{2},$$
but this contradicts Equation (10.9.1). □

Notes

Exercises

Chapter 11

Pretty Good State Transfer

In this chapter we describe the known examples of graph on which pretty good state transfer occurs. The list is not extensive. We determine the paths that do admit pgst and we study one class of trees.

For paths, the characterization depends in a surprising way on the prime factors of $n+1$. Our treatment follows Godsil, Kirkland, Severini and Smith [37]. Burgath [15] showed that pgst occurs on paths of length n when n is prime and Vinet and Zhedanov [57] derive related results.

11.1 PGST on Paths

The eigenvalues θ_r of the path are given by

$$\theta_r = 2\cos\Big(\frac{\pi r}{n+1}\Big).$$

In consequence, θ_r is a polynomial with rational coefficients of degree r in θ_1. We also set $\theta_0 = 2$.

11.1.1 Lemma. *The numbers $\theta_0, \ldots, \theta_d$ are linearly independent over $\mathbb{Q}$ if and only if the degree of the algebraic integer θ_1 is greater than d.* □

11.1.2 Theorem. *If $n = p-1$ or $2p-1$, where p is prime, or if $n = 2^m - 1$ then we have pgst on P_n.*

Proof. Let $\theta = 2\cos\big(\frac{\pi}{n+1}\big)$ and set $\zeta = e^{i\pi/(n+1)}$. Then $\theta \in \mathbb{Q}(\zeta)$ and ζ is a root of the quadratic

$$x^2 - 2\theta x + 1.$$

So the index of $\mathbb{Q}(\theta)$ in $\mathbb{Q}(\zeta)$ is at most two. If $n \geq 3$ though, θ is real and ζ is not. So the index is two. The degree of ζ is $\phi(2n+2)$, where ϕ is Euler's function, and therefore the degree of θ is $\phi(2n+2)/2$.

If $n = p-1$ where p is prime then

$$\frac{\phi(2(n+1))}{2} = \frac{\phi(2p)}{2} = \frac{\phi(p)}{2} = \frac{p-1}{2}.$$

If $n = 2p-1$ for a prime p, then

$$\frac{\phi(2(n+1))}{2} = \frac{\phi(4p)}{2} = \phi(p) = p-1.$$

If $n = 2^m - 1$, then $\phi(2(n+1))/2 = 2^{m-1}$. Therefore in each of these three cases the positive eigenvalues of P_n are linearly independent over $\mathbb{Q}$, and we have pgst. □

11.2 Phases and Pretty Good State Transfer

We show that, aside from the cases already listed, pretty good state transfer does not occur on a path.

Our first result is an extension of Lemma 1.8.2.

11.2.1 Lemma. *Assume X is bipartite and we have pretty good state transfer from a to b. Suppose $U(t)e_a$ is close to γe_b. If a and b lie in the same color class, then γ is close to 1 or -1. If a and b lie in different color classes, γ is close to i or $-i$.*

Proof. Suppose X is bipartite and let D be the diagonal matrix such that $D_{u,u}$ is 1 or -1 according as u is in the first or second part of the bipartition. Then $DAD = -A$ and if $U(t)e_a \approx \gamma e_b$, then

$$\gamma De_b \approx DU(t)D\, De_a = U(-t)De_a$$

But e_a and e_b are eigenvectors for D with eigenvalues 1 or -1; the eigenvalues are equal if and only if u and v are in the same part. So there is a sign factor $\sigma_{a,b}$ and

$$\gamma e_b \approx \sigma_{a,b} U(-t)e_a.$$

Accordingly

$$U(t)e_b \approx \gamma^{-1}\sigma_{a,b}e_a.$$

Since $U(t)e_b \approx \gamma e_a$, we conclude that

$$\gamma \approx \gamma^{-1}\sigma_{a,b}$$

Therefore $\gamma \approx \pm 1$ if a and b are in the same part, and $\gamma \approx \pm i$ if they are not. □

Let F denote the permutation matrix of order $n \times n$ such that $Fe_r = e_{n+1-r}$ for all r. Let $E_1, \dots, E_n$ be the idempotents in the spectral decomposition of the path P_n. Then

$$F = \sum_{r=1}^{n} (-1)^{r-1} E_r.$$

If we have pgst at time τ then

$$U(\tau) \approx \gamma F$$

and therefore

$$1 = \det U(\tau) \approx \gamma^n \det(F) = \gamma^n (-1)^{\lfloor n/2 \rfloor}.$$

Appealing to Lemma 11.2.1, this yields three cases:

(a) $n \equiv 1 \bmod 4$: then $(-1)^{\lfloor n/2 \rfloor} = 1$ and $\gamma \approx 1$

(b) $n \equiv 3 \bmod 4$: then $(-1)^{\lfloor n/2 \rfloor} = -1$ and $\gamma \approx -1$

(c) n is even: here $i^n = (-1)^{n/2}$ and $\gamma \approx \pm i$.

If pgst occurs then $U(t)$ gets arbitrarily close to γF. This means that

$$e^{i\theta_r t} \approx (-1)^{r-1}\gamma \tag{11.2.1}$$

for $r = 1, \dots, n$. Set $m = \lfloor n/2 \rfloor$.

11.2.2 Lemma. *Assume $\gamma = \pm 1$ if n is odd and $\pm i$ if n is even. For the path P_n, if $e^{i\theta_r t} \approx (-1)^{r-1}\gamma$ for $r = 1, \dots, m$ then $e^{i\theta_r t} \approx (-1)^{r-1}\gamma$ for all r and $U(t) \approx \gamma F$.*

Proof. Assume $e^{i\theta_r t} \approx (-1)^{r-1}\gamma$ for $r = 1, \dots, m$. Since paths are bipartite, $\theta_{n+1-r} = \theta_r$, and therefore

$$e^{i\theta_{n+1-r}t} = e^{-i\theta_r t} \approx (-1)^{r-1}\gamma^{-1}.$$

So for pgst we need

$$(-1)^{n-r}\gamma = (-1)^{r-1}\gamma^{-1},$$

or equivalently

$$\gamma^2 = (-1)^{n-1}.$$

As this holds for our choice of γ, we are done. □

11.3 No PGST on Paths

We show that, in the cases not listed in Section 11.1, pgst does not occur on P_n. If $n+1$ is not a power of two, then it is divisible by an odd prime p. If also n is not a prime or twice a prime, then $n = mp$ where $m \geq 4$, and thus our next result completes the classification of the paths that admit pgst.

11.3.1 Theorem. *If $n = mp - 1$ where p is odd and $m \geq 3$, then pgst does not occur on P_n.*

Proof. Suppose $n + 1 = mp$ where p is odd. Then

$$1 + 2\sum_{r=1}^{\frac{p-1}{2}} (-1)^r \cos\left(\frac{\pi r}{p}\right) = 0.$$

If we multiply this by $\cos\left(\frac{\pi}{n+1}\right)$ we get

$$\cos\left(\frac{\pi}{n+1}\right) + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r \left[\cos\left(\frac{\pi(mr+1)}{n+1}\right) + \cos\left(\frac{\pi(mr-1)}{n+1}\right)\right] = 0$$

which yields a relation on eigenvalues:

$$\theta_1 + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r \theta_{mr+1} + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r \theta_{mr-1} = 0.$$

Similarly if we multiply our first equation by $\cos\left(\frac{2\pi}{n+1}\right)$ we derive:

$$\theta_2 + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r \theta_{mr+2} + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r \theta_{mr-2} = 0.$$

If we subtract the last equation from the previous one, we find that

$$(\theta_1 - \theta_2) + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r (\theta_{mr+1} - \theta_{mr+2}) + \sum_{r=1}^{\frac{p-1}{2}} (-1)^r (\theta_{mr-1} - \theta_{mr-2}) = 0.$$

Denote the three terms on the left by D, E and F respectively. If we have pgst, we have a sequence of times $(t_k)_{k\geq 0}$ such that $e^{i\theta_r t_k} \to (-1)^{r-1}\gamma$, and so

$$e^{i(\theta_s - \theta_{s+1})t_k} \to -1.$$

Therefore $e^{iDt_k} \to -1$ while e^{iEt_k} and e^{iEt_k} both tend to 1 or to -1. Thus

$$e^{i(D+E+F)t_k} \to -1,$$

which is impossible since $D + E + F = 0$. □

11.3.2 Theorem. *If $n = 3k + 2$ then pretty good state transfer does not occur on P_n if k is even or is congruent to 3 mod 4.*

Proof. Assume by way of contradiction that we do have pgst. Hence there is a time t such that (11.2.1) holds.

Now since $n \equiv 2 \bmod 3$, we have

$$\theta_1 = \theta_k + \theta_{k+2}$$

and therefore

$$e^{i\theta_1 t} \approx (-1)^{2k} e^{i\theta_k t} e^{i\theta_{k+2} t}.$$

This implies that

$$\gamma = \gamma^2$$

and so $\gamma = 1$ and $n \equiv 1$ modulo 4. □

11.4 Path Laplacians

In the following sections we use the transition operator

$$U(t) := \exp(it(\Delta - A))$$

and determine the cases where pgst occurs on the path.

We will see that we have pgst using the Laplacian on P_4 and that P_2 and P_4 are the only cases where we get pst or pgst using the Laplacian on paths.

We denote the eigenvalues of the Laplacian of the path by $\theta_0, \ldots, \theta_{n-1}$, where $\theta_0 = 0$ and $\theta_i \leq \theta_{i+1}$. We recall from Section 10.5 that

$$\theta_r = 2 - 2\cos\left(\frac{\pi r}{n}\right), \qquad (r = 0, \ldots, n-1).$$

We use $E_0, \ldots, E_{n-1}$ to denote the corresponding idempotents in the spectral decomposition. Hence

$$E_0 = \frac{1}{n}J.$$

From Lemma 10.5.2 we have

$$(E_r)_{j,k} = \frac{2}{n}\cos\left(\frac{(2j-1)r\pi}{2n}\right)\cos\left(\frac{(2k-1)r\pi}{2n}\right).$$

Let F denote the permutation matrix such that $Fe_r = e_{n+1-r}$. Since F is an automorphism of P_n, it commutes with L and since the eigenvalues of L are simple it follows that F is a polynomial in L. Therefore F is a linear combination of the idempotents E_r; the coefficients in this linear combination are the eigenvalues of F (and there they are all ± 1). Since $FE_r = (-1)^r E_r$ we conclude that

$$F = \sum_{r=0}^{n-1} (-1)^r E_r.$$

Now

$$U(t)_{1,n} = \sum_{r=0}^{n-1} e^{it\theta_r}(E_r)_{1,n}.$$

Since $(E_r)_{1,n} = (-1)^r (E_r)_{1,1}$ and since $\sum_e (E_r)_{1,1} = 1$, we see that $U(t)_{1,n}$ is a convex combination of complex numbers of norm 1. If $|U(t)_{1,n}| = 1$, it follows that complex numbers $(-1)^r e^{it\theta_r}$, for $r = 0, \dots, n-1$, are all equal. As $\theta_0 = 0$, this implies that these numbers are all equal to 1 and further that

$$U(t) = \sum_r (-1)^r E_r = F.$$

Similarly we deduce that if $|U(t)_{1,n}| \approx 1$ then $U(t) \approx F$.

If $n \geq 6$ and is not an odd prime or a power of two, the following shows that we do not get pgst using the Laplacian of P_n.

11.4.1 Theorem. *If $n = mk$ where k is odd and $m \geq 2$, then we do not have pgst on P_n using the Laplacian.*

Proof. Our argument is modelled on the proof of Theorem 11.3.1. We have the identity

$$1 + 2\sum_{r=1}^{\frac{k-1}{2}} (-1)^r \cos\left(\frac{\pi r}{k}\right) = 0.$$

If we multiply this by $\cos\left(\frac{\pi}{n}\right)$ we get

$$\cos\left(\frac{\pi}{n}\right) + \sum_{r=1}^{\frac{k-1}{2}} (-1)^r \left[\cos\left(\frac{\pi(mr+1)}{n}\right) + \cos\left(\frac{\pi(mr-1)}{n}\right)\right] = 0;$$

similarly if we multiply both sides of our identity by $\cos\left(\frac{2\pi}{n}\right)$ we find that

$$\cos\left(\frac{2\pi}{n}\right) + \sum_{r=1}^{\frac{k-1}{2}} (-1)^r \left[\cos\left(\frac{\pi(mr+2)}{n}\right) + \cos\left(\frac{\pi(mr-2)}{n}\right)\right] = 0.$$

If we subtract the first equation from the second and then translate the cosines to eigenvalues, we find that

$$(\theta_1 - \theta_2) + \sum_{r=1}^{\frac{k-1}{2}} (-1)^r (\theta_{mr+1} - \theta_{mr+2}) + \sum_{r=1}^{\frac{k-1}{2}} (-1)^r (\theta_{mr-1} - \theta_{mr-2}) = 0.$$

Arguing as in the proof of Theorem 11.3.1, we arrive at a contradiction. □

11.4.2 Lemma. *We have pgst on P_4 using the Laplacian.*

Proof. The characteristic polynomial of the Laplacian of P_4 is

$$t(t-2)(t^2-4t+2)$$

and so the eigenvalues of the Laplacian are

$$0,\ 2-\sqrt{2},\ 2,\ 2+\sqrt{2}$$

We want $U(t)$ to get arbitrarily close to $E_0 - E_1 + E_2 - E_3$ Hence we need a sequence of times $(t_k)_{k\geq 0}$ such that

$$e^{(2-\sqrt{2})it_k},\ e^{(2+\sqrt{2})it_k} \to -1$$

while

$$e^{2it_k} \to 1.$$

Suppose we have sequence of pairs (a_k, b_k) of integers such that a_k/b_k converges to $2-\sqrt{2}$. Then

$$b_k(2-\sqrt{2}) \approx a_k$$

and

$$b_k(2+\sqrt{2}) = b_k(4-(2-\sqrt{2})) \approx 4b_k - a_k$$

This means that if a_k is odd then we may choose $t_k = b_k\pi$. If we set

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix}, \quad \alpha_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and define $\alpha_k := M^k\alpha_0$, then

$$\frac{(\alpha_k)_1}{(\alpha_k)_2} \to \sqrt{2}-1$$

as $k \to \infty$ and so we may take $b_k = (\alpha_k)_2 - (\alpha_k)1$ and $a_k = (\alpha_k)_2$. Since M is congruent mod 2 to

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we see that $(\alpha_k)_1$ is odd when k is odd. We conclude that we have pgst on P_4.

11.5 Double Stars

In this section we follow Fan and Godsil [27] `http://arxiv.org/abs/1206.0082`. The *double star* $S_{k,\ell}$ is the tree obtained from the stars $K_{1,k}$ and $K_{1,\ell}$ by adding an edge joining the two central vertices. We assume k and ℓ are both positive. For the proof of the next result we refer you to the above paper.

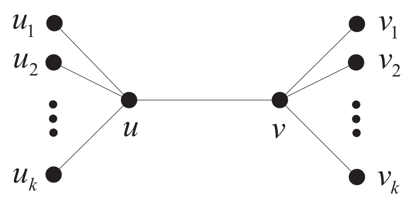

Figure 11.1: The double star $S_{k,k}$

11.5.1 Theorem. *Perfect state transfer does not occur on the double star.* □

11.5.2 Theorem. *Suppose a and b are vertices of degree in one in $S_{2,\ell}$ adjacent to the vertex of valency three. If $\ell \neq 2$, we have pretty good state transfer from a to b.*

Proof. Let c be the common neighbour of a and b, and let d be the third neighbour of c. Then the partition

$$\pi = \{\{a\}, \{b\}, \{c\}, \{d\}, N(d) \setminus \{c\}$$

is equitable. Let Y be the symmetrized quotient graph of X relative to π, and let B be the adjacency matrix of Y. Thus

$$B = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & \sqrt{\ell} \\ 0 & 0 & 0 & \sqrt{\ell} & 0 \end{pmatrix}$$

and

$$\phi(B, t) = t(t^4 - (\ell + 3)t^2 + 2\ell).$$

The eigenvalues of B are

$$\begin{aligned}\theta_1 &= 0,\\ \theta_2 &= \sqrt{\frac{1}{2}(\ell+3+\sqrt{\ell^2-2\ell+9})},\\ \theta_3 &= -\sqrt{\frac{1}{2}(\ell+3+\sqrt{\ell^2-2\ell+9})},\\ \theta_4 &= \sqrt{\frac{1}{2}(\ell+3-\sqrt{\ell^2-2\ell+9})},\\ \theta_5 &= -\sqrt{\frac{1}{2}(\ell+3-\sqrt{\ell^2-2\ell+9})}.\end{aligned}$$

Let F be the permutation matrix that represents the automorphism of Y that swaps a and b (and leaves the other vertices fixed). Since the eigenvalues of B are distinct since F commutes with B, we conclude that F is a polynomial in B and therefore it is a linear combination of the spectral idempotents of B. Straightforward calculation yields that

$$F = -E_1 + E_2 + E_3 + E_4 + E_5,$$

where

$$E_1 = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & 0 & 0\\ -1 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\end{pmatrix}.$$

If $U_B(t) \approx \gamma F$, then

$$1 = \det(U_B(t)) \approx \gamma^5 \det(F) = -\gamma^5.$$

So $U_B(t) \approx -F$ and hence

$$(e^{it\theta_1}, e^{it\theta_2}, e^{it\theta_3}, e^{it\theta_4}, e^{it\theta_5}) \approx (1, -1, -1, -1, -1).$$

Since $\theta_1 = 0$ and $\theta_3 = -\theta_2$ and $\theta_5 = -\theta_4$, we conclude that we have pgst if there is sequence of times t_r such that both $e^{i\theta_2}$ and $e^{i\theta_4}$ tend to -1.

To prove this we will apply Kronecker's theorem and so, as a first step, we verify that θ_2 and θ_4 are linearly independent over $\mathbb{Q}$. If θ_2/θ_4 is rational then so is

$$\frac{\theta_2^2}{\theta_4^2} = \frac{\ell+3+\sqrt{\ell^2-2\ell+9}}{\ell+3-\sqrt{\ell^2-2\ell+9}}.$$

This can hold only if $\sqrt{\ell^2-2\ell+9}$ is an integer, that is, if $\ell = 2$. Since θ_2 and θ_4 are irrational, we conclude by Kronecker's theorem (Theorem 8.5.2) that have pgst from a to b. □

11.5.3 Theorem. *Let a and b be the vertices of degree $k+1$ in the double star $S_{k,k}$. We have pretty good state transfer from a to b if and only if $1+4k$ is not a perfect square.*

Proof. Let A be the adjacency matrix of $S_{k,k}$ and let a and b be the central vertices of degree $k+1$. A standard calculation yields that

$$U(t)_{a,b} = i((1-2\beta)\sin(\alpha t) + 2\beta\sin(1-\alpha)t$$

where

$$\alpha = \frac{1}{2}(1+\sqrt{1+4k}), \qquad \beta = \frac{k}{1+4k+\sqrt{1+4k}}.$$

Observe that $\beta \le 1/4$, and so the above expression shows that $-iU(t)$ is a convex combination of $\sin(\alpha t)$ and $\sin(1-\alpha)t$. It follows that $|U(t)_{a,b}| \approx 1$ if and only if $\sin(\alpha t)$ and $\sin(1-\alpha)t$ are both close to 1, or both close to -1. Or, equivalently if $\sin(\alpha t)\sin(1-\alpha)t \approx 1$.

Now, from the distant past, recall that

$$\cos(t) = \cos(\alpha t)\cos(1-\alpha)t - \sin(\alpha t)\sin(1-\alpha)t;$$

since if $\sin^2(\alpha t) \approx 1$ we have $\cos(\alpha t) \approx 0$, we conclude that if

$$\sin(\alpha t)\sin(1-\alpha)t \approx 1$$

then $\cos(t) \approx -1$. Thus to show pgst occurs, we must find a sequence of times $(t_r)_{r\ge 0}$ such that

$$\lim_{r\to\infty} \cos(t) = -1, \quad \lim_{r\to\infty} \sin^2(\alpha t) = 1.$$

If $4k+1$ is not a perfect square, this is another appplication of Kronecker's theorem.

If $4k+1$ is a perfect square the eigenvalues of $S_{k,k}$ are integers and so the graph is periodic. Hence if pgst occurs, then pst occurs, which contradicts Theorem 11.5.1.

Notes

Exercises

Chapter 12

Joins and Products

We have seen that the Cartesian product of graphs is intimately connected with state transfer. In this chapter we will investigate how other standard graph theoretic operations can be used to get examples of perfect state transfer. (Another goal of this chapter is to provide a wide range of examples where perfect state transfer occurs.)

We start with joins. If X and Y are graphs their *join* $X+Y$ is the graph we get by taking a copy of X and a copy of Y and joining each vertex in X to each vertex in Y. Angeles-Canul et al. [4, 3] and the Ge et al. [30] provide many interesting results on perfect state transfer in joins. Here we will focus on the joins of two regular graphs.

The second operation we will study is the *direct product* $X \times Y$ of graphs X and Y. For our purposes the simplest way to define this is to state that

$$A(X \times Y) = A(X) \otimes A(Y).$$

Roughly speaking, there are many graphs that can be expressed as the edge-disjoint unions of direct products and, in some cases, we can make use of this structure.

12.1 Eigenvalues and Eigenvectors of Joins

Let X be a k-regular graph on m vertices and let Y be an ℓ-regular graph on n vertices. In this section we describe the spectral decomposition of their join $Z := X + Y$. Note that the join has an equitable partition π with cells $(V(X), V(Y))$. Set $A = A(X)$ and $B = A(Y)$ and let $\hat{A}$ denote the adjacency matrix of Z. Then

$$\hat{A} = \begin{pmatrix} A & J \\ J^T & B \end{pmatrix}$$

and the adjacency matrix of the quotient Z/π is

$$Q = \begin{pmatrix} k & n \\ m & \ell \end{pmatrix}.$$

Its eigenvalues are the zeros of the quadratic

$$t^2 - (k+\ell)t + (k\ell - mn),$$

thus they are

$$\frac{1}{2}(k + \ell \pm \sqrt{(k-\ell)^2 + 4mn}).$$

We denote them by μ_1 and μ_2, with $\mu_1 > \mu_2$. Since

$$(Q - \mu_1 I)(Q - \mu_2 I) = 0$$

we see that the columns of $Q - \mu_2 I$ are eigenvectors for Q with eigenvalue μ_1, and the columns of $Q - \mu_1 I$ are eigenvectors for Q with eigenvalue μ_2. Hence the eigenvectors of $\hat{A}$ belonging to μ_1 and μ_2 respectively can be written in partitioned form:

$$\begin{pmatrix} (k-\mu_2)\mathbf{1} \\ m\mathbf{1} \end{pmatrix}, \quad \begin{pmatrix} (k-\mu_1)\mathbf{1} \\ m\mathbf{1} \end{pmatrix}.$$

The remaining eigenvectors of $\hat{A}$ can be taken to be orthogonal to these two vectors, and therefore such eigenvectors must sum to zero on $V(X)$ and $V(Y)$. If x is an eigenvector for X orthogonal to $\mathbf{1}$ with eigenvalue λ, then

$$\begin{pmatrix} x \\ 0 \end{pmatrix}$$

is an eigenvector for Z with eigenvalue λ. Similarly if y is an eigenvector for Y orthogonal to $\mathbf{1}$, then

$$\begin{pmatrix} 0 \\ y \end{pmatrix}$$

is an eigenvector for $\hat{A}$ (with the same eigenvalue as y). As a consequence, we have just exhibited a full basis of eigenvectors of $\hat{A}$ that depends only on the eigenvectors of A and B, and the parameters k, ℓ, m and n.

12.2 Spectral Idempotents for Joins

We are going to construct a refinement of the spectral decomposition of the join Z of X and Y. (If X and Y are connected and have no eigenvalue in common, this will be the actual spectral decomposition of Z.) This decomposition will, in large part, be built from the spectral decompositions of X and Y.

If X is connected, we will use the spectral decomposition of A:

$$A = \sum_{r=0}^{d} \theta_r E_r$$

where $\theta_0 = k$ and $E_0 = \frac{1}{m}J$. If X is not connected, then k has multiplicity greater than one, and we can choose a basis for its eigenspace formed by the all ones vector $\mathbf{1}$, and other vectors which are constant on each component and whose all entries sum to zero. The idempotent belonging to k can then be written as the sum of $\frac{1}{m}J$ and a second idempotent. Now we have a refinement of the spectral decomposition of X, with one extra term. We will still write this in the form above, with the understanding that $\theta_1 = \theta_0$. A similar fuss can be made if Y is not connected; we write its decomposition as

$$B = \sum_{s=0}^{f} \nu_s F_s.$$

If $Az = \theta z$ and $\mathbf{1}^T z = 0$, then

$$\hat{A} \begin{pmatrix} z \\ 0 \end{pmatrix} = \theta \begin{pmatrix} z \\ 0 \end{pmatrix}.$$

Similarly if $Bz = \theta z$ and $\mathbf{1}^T z = 0$, then

$$\hat{A} \begin{pmatrix} 0 \\ z \end{pmatrix} = \theta \begin{pmatrix} 0 \\ z \end{pmatrix}.$$

We see that $n+m-2$ of the eigenvalues of $X+Y$ are eigenvalues of X and eigenvalues of Y.

Define

$$\hat{E}_r = \begin{pmatrix} E_r & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{F}_s = \begin{pmatrix} 0 & 0 \\ 0 & F_s \end{pmatrix}$$

and let N_1 and N_2 be the projections belonging to the eigenvalues μ_1 and μ_2 of Z. Then we have a spectral decomposition for $\hat{A} = A(Z)$:

$$\hat{A} = \mu_1 N_1 + \mu_2 N_2 + \sum_{r>0} \theta_r \hat{E}_r + \sum_{s>0} \nu_s \hat{F}_s. \tag{12.2.1}$$

We determined μ_1 and μ_2 in terms of k, ℓ, m and n in the previous section. Since $\sum_r E_r = I$ and $\sum_s F_s = I$ we have

$$\sum_{r>0} \hat{E}_r = \begin{pmatrix} I - \frac{1}{m}J & 0 \\ 0 & 0 \end{pmatrix}, \quad \sum_{s>0} \hat{F}_s = \begin{pmatrix} 0 & 0 \\ 0 & I - \frac{1}{n}J \end{pmatrix}$$

and since the sum of the idempotents in (12.2.1) is I, it follows that

$$N_1 + N_2 = I - \begin{pmatrix} I - \frac{1}{m}J & 0 \\ 0 & I - \frac{1}{n}J \end{pmatrix}.$$

The idempotent N_1 represents projection onto the span of the eigenvector

$$\begin{pmatrix} (k-\mu_2)\mathbf{1} \\ m\mathbf{1} \end{pmatrix}$$

and consequently

$$N_1 = c \begin{pmatrix} (k-\mu_2)^2 J_{m,m} & m(k-\mu_2)J_{m,n} \\ m(k-\mu_2)J_{n,m} & m^2 J_{n,n} \end{pmatrix}$$

where c is determined by the constraint $\operatorname{tr}(N_1) = 1$. This means that

$$c^{-1} = m(k-\mu_2)^2 + m^2 n = m((k-\mu_2)^2 + mn).$$

If we set

$$\Delta = (k-\ell)^2 + 4mn$$

then, after some calculation, we find that

$$(k-\mu_2)^2 + mn = \sqrt{\Delta}(k-\mu_2).$$

Hence $c^{-1} = m\sqrt{\Delta}(k-\mu_2)$. We can carry out similar calculations for N_2, with the result that

$$N_1 = \frac{1}{m\sqrt{\Delta}(k-\mu_2)} \begin{pmatrix} (k-\mu_2)^2 J_{m,m} & m(k-\mu_2)J_{m,n} \\ m(k-\mu_2)J_{n,m} & m^2 J_{n,n} \end{pmatrix},$$

$$N_2 = \frac{1}{m\sqrt{\Delta}(\mu_1-k)} \begin{pmatrix} (k-\mu_1)^2 J_{m,m} & m(k-\mu_1)J_{m,n} \\ m(k-\mu_1)J_{n,m} & m^2 J_{n,n} \end{pmatrix}.$$

12.3 The Transition Matrix of a Join

Suppose Z is the join $X+Y$ and a and b are two vertices in X. We want to determine when we have perfect state transfer from a to b in Z. We note that if we do have perfect state transfer from a to b at time t, then $U_Z(t)_{a,u}=0$ for all vertices u of Y and $U_Z(t)_{a,a}=0$.

12.3.1 Lemma. *Assume Z is the join of graphs X and Y. If $a,b\in V(X)$ and $y\in V(Y)$, then*

$$U_Z(t)_{a,y}=\frac{1}{\sqrt{\Delta}}(\exp(i\mu_1 t)-\exp(i\mu_2 t))$$

and

$$U_Z(t)_{a,b}-U_X(t)_{a,b}=\frac{1}{m}\left(\frac{k-\mu_2}{\sqrt{\Delta}}\exp(i\mu_1 t)-\frac{k-\mu_1}{\sqrt{\Delta}}\exp(i\mu_2 t)-\exp(ikt)\right).$$

Proof. Since $(\hat{E}_r)_{a,y}=(\hat{F}_r)_{a,y}=0$ we have

$$U_Z(t)_{a,y}=\exp(i\mu_1 t)(N_1)_{a,y}+\exp(i\mu_2 t)(N_2)_{a,y}=\frac{1}{\sqrt{\Delta}}(\exp(i\mu_1 t)-\exp(i\mu_2 t)).$$

From our spectral decomposition,

$$U_Z(t)_{a,b}=\frac{k-\mu_2}{m\sqrt{\Delta}}\exp(i\mu_1 t)-\frac{k-\mu_1}{m\sqrt{\Delta}}\exp(i\mu_2 t)+\sum_{r>0}(E_r)_{a,b}\exp(i\theta_r t).$$

Since X is regular,

$$U_X(t)=\frac{1}{m}\exp(ikt)J_n+\sum_{r>0}\exp(i\theta_r t)E_r,$$

from which our second expression follows. □

Therefore $U_Z(t)_{a,y}=0$ if and only if $\exp(it(\mu_1-\mu_2))=1$, that is, if and only if for some integer c,

$$t=\frac{2c\pi}{\mu_1-\mu_2}=\frac{2c\pi}{\sqrt{\Delta}}.$$

Since $(k-\mu_2)-(k-\mu_1)=\sqrt{\Delta}$, we find that for these values of t we have

$$U_Z(t)_{a,b}-U_X(t)_{a,b}=\frac{1}{m}(\exp(i\mu_1 t)-\exp(ikt)).$$

12.4 Joins with K_2 and $\overline{K_2}$

We use the results of the previous section to construct graphs with perfect state transfer. Our first result is due to Angeles-Canul et al [4]. If q is a rational number such that

$$q = 2^k(a/b),$$

where a and b are odd, we define $|q|_2$ to be 2^{-k}. (This is the 2-adic norm on $\mathbb{Q}$. Note that larger powers of 2 have smaller norms.)

12.4.1 Lemma. *(THERE IS SOMETHING WRONG HERE... $\ell^2 + 8n$ must be integer...) If $X = \overline{K_2}$ and Y is ℓ-regular on n vertices, we have perfect state transfer in $X + Y$ between the two vertices of X if and only if*

(a) $\ell = 0$, *or*

(b) $\ell > 0$ *and* $n = \ell(\ell + s)/2$

(c) s *and* n *are even and* $4|\ell$,

(d) $|\ell/s|_2 < 1$.

Proof. As above, $U_{X+Y}(t)_{a,y} = 0$ if and only if $\exp(it(\mu_1 - \mu_2)) = 1$.

Since $U_X(t)_{a,a} = 1$ for all t, we see that $U_{X+Y}(t)_{a,a} = 0$

$$-1 = \frac{1}{2}(\exp(i\mu_1 t) - \exp(ikt)) = \frac{1}{2}(\exp(i\mu_1 t) - 1)$$

and this holds if and only if $\exp(it\mu_1) = -1$.

It follows that if perfect state transfer occurs at time t, then $\exp(it\mu_1)$ and $\exp(it\mu_2)$ both equal -1, and consequently

$$1 = \exp(it(\mu_1 + \mu_2)) = \exp(it\ell).$$

Hence either $\ell = 0$ or $t = 2d\pi/\ell$ for some integer d, from which we deduce that $\sqrt{\Delta}$ is rational and Δ is a perfect square.

If $\ell = 0$, then $\mu_1 = \sqrt{2n}$ and $\exp(it\mu_1) = -1$ when $t\mu_1$ is an odd multiple of π.

Assume $\ell > 0$. If $\ell^2 + 8n$ is a perfect square, then when t is an even multiple of $\pi/\sqrt{\Delta}$ we have

$$\exp(it\mu_1) = \exp(it\mu_2)$$

and when t is an even multiple of π/ℓ we have

$$\exp(it\mu_1) = \exp(-it\mu_2).$$

Let δ denote the greatest commmon divisor of $\sqrt{\Delta}$ and ℓ. The last pair of equations hold provided $t/2\pi$ is an integer multiple of $1/\delta$. We get perfect state transfer if and only if

$$\exp(2\pi i\mu_1/\delta) = -1.$$

Now

$$\frac{2\mu_1}{\delta} = \frac{\ell + \sqrt{\Delta}}{\delta}$$

and so we have perfect state transfer if and only if Δ is a perfect square and $(\ell + \sqrt{\Delta})/\delta$ is an odd integer.

We see that $\ell^2 + 8n$ is a perfect square if and only if $8n = 4s(\ell + s)$ for some integer s such that $s(\ell + s)$ is even, i.e., so that s is odd if ℓ is. Then

$$\sqrt{\Delta} = \ell + 2s, \quad \mu_1 = \frac{1}{2}(\ell + \ell + 2s) = \ell + s$$

and δ is the gcd of ℓ and $2s$. Further

$$\frac{\ell + \sqrt{\Delta}}{\delta} = \frac{2\ell + 2s}{\delta}$$

from which it follows that perfect state transfer occurs if and only if $2s/\delta$ is odd.

If ℓ is odd or s is odd, then δ is odd, and so for perfect state transfer both ℓ and s must be even, and therefore n is even. For $2s/\delta$ to be odd we require that δ is divisible by four, hence $4|\ell$. Further ℓ/δ must be even, equivalently $|\ell/s|_2 < 1$. □

As a simple example, take Y to be $C_5 \otimes C_6$ (due to Angeles-Canul et al). Then $n = 30$, $\ell = 4$ and $s = 6$ and so all conditions of the theorem hold, and therefore we have perfect state transfer on $\overline{K_2} + Y$. This was the first example of a graph with perfect state transfer which is not periodic. (We leave the proof that is not periodic as an exercise. If you choose to do it by hand, note that any eigenvalue of C_5 or C_6 that has an eigenvector orthogonal to $\mathbf{1}$ is an eigenvalue of the join.)

Angeles-Canul et al also prove the following.

12.4.2 Lemma. *Suppose Y is an ℓ-regular graph on n vertices. Then there is perfect state transfer in K_2+Y between the vertices of K_2 if and only if:*

(a) $n = s(\ell-1+s)/2$ for some even integer s, and

(b) $|\frac{\ell+s+1}{\ell+2s}|_2 > 1$.

Proof. We sketch the proof. As before, $U_{X+Y}(t)_{a,y} = 0$ if and only if

$$1 = \exp(it(\mu_1-\mu_2)) = \exp(it\sqrt{\Delta})$$

and so $t\sqrt{\Delta}$ must be an even multiple of π. At these times

$$U_{X+Y}(t)_{a,a} = U_X(t)_{a,a} + \frac{1}{2}(\exp(i\mu_1 t) - \exp(ikt)).$$

Since $X = K_2$,

$$U_X(t) = \cos(t) = \frac{1}{2}(\exp(it) - \exp(-it))$$

and since $k = 1$ we have

$$U_{X+Y}(t)_{a,a} = \frac{1}{2}(\exp(i\mu_1 t) + \exp(-it)).$$

Therefore we have perfect state transfer between the two vertices of X at time t if and only if

$$\exp(it\sqrt{\Delta}) = 1, \quad \exp(it(\mu_1+1)) = -1.$$

Accordingly there are integers r and s such that

$$t\sqrt{\Delta} = 2r\pi, \quad t(\mu_1+1) = (2s+1)\pi,$$

from which it follows that

$$\frac{\mu_1+1}{\sqrt{\Delta}} = \frac{2s+1}{2r}$$

and hence $\sqrt{\Delta}$ and μ_1 are integers.

Now $(\ell-1)^2+8n$ is a perfect square if and only if there is an integer s such that $s\ell$ is even and

$$n = \frac{1}{2}s(\ell-1+s).$$

In this case

$$\sqrt{\Delta} = \ell - 1 + 2s, \quad \mu_1 + 1 = \ell + s + 1. \qquad \square$$

A sufficient condition for (b) to hold is that $s \equiv 0$ modulo 4 and $\ell \equiv 1$ modulo 8. However other solutions are possible, for example $s \equiv 6$ and $\ell \cong 5$ modulo 8. (I suspect an exact description in terms of congruence classes might be complicated.)

Ge et al. [30] give results for the lexicographic product.

12.5 Irrational Periods and Phases

In our examples of periodic vertices, the period has been rational. We use the results of the Section 12.3 to construct examples where the period is irrational. (The associated phases are irrational too.)

A graph X on n vertices is a *cone* over a graph Y if there is a vertex u of X with degree $n-1$ such that $X \setminus u \cong Y$. (Equivalently X is isomorphic to $K_1 + Y$.) We say u is the *conical vertex*, or the *apex* of the cone.

12.5.1 Lemma. *Suppose Y is an ℓ-regular graph on n vertices and let Z be the cone over Y. The Z is periodic at the conical vertex with period $2\pi/\sqrt{\ell^2 + 4n}$.*

Proof. We view Z as the join of X and Y, with $X = K_1$. If a is the conical vertex, then $|U_Z(t)_{a,a}| = 1$ if and only if $U_Z(t)_{a,y} = 0$ for all y in $V(Y)$. This holds if and only if $t/2\pi$ is an integer multiple of Δ, where $\Delta = \sqrt{\ell^2 + 4n}$. $\square$

We have

$$U(t)_{a,a} = \sum_r e^{it\theta_r} (E_r)_{a,a}$$

where $(E_r)_{a,a} \geq 0$ and $\sum_r (E_r)_{a,a} = 1$. Hence $|U(t)_{a,a}| = 1$ if and only if $e^{it\theta_r} = e^{it\theta_1}$ for all r, and therefore

$$U(t)_{a,a} = e^{it\theta_1}.$$

So for a periodic cone the phase factor at the period is $e^{it\mu_1}$, where

$$\mu_1 = \frac{1}{2}(\ell + \sqrt{\ell^2 + 4n}).$$

Now it follows that for some integer c

$$t\mu_1 = \frac{2c\pi}{\sqrt{\ell^2 + 4n}} \frac{1}{2}(\ell + \sqrt{\ell^2 + 4n}) = \frac{c\pi\ell}{\sqrt{\ell^2 + 4n}} + c\pi.$$

In all currently known cases where we have perfect state transfer, the phase factor is a root of unity. The calculations we have just completed show that if $\ell^2 + 4n$ is not a perfect square, we have periodicity on the cone over Y with phase factor not a root of unity.

12.6 The Direct Product

If X and Y are graphs then their *direct product* $X \times Y$ is the graph with adjacency matrix

$$A(X) \otimes A(Y).$$

12.6.1 Lemma. *Suppose X and Y are graphs with respective adjacency matrices A and B and suppose A has spectral decomposition*

$$A = \sum_r \theta_r E_r.$$

Then

$$U_{X\times Y}(t) = \sum_r E_r \otimes U_Y(\theta_r t).$$

Proof. First,

$$A \otimes B = \sum_r \theta_r E_r \otimes B$$

and since the matrices $E_r \otimes B$ commute,

$$U_{X\times Y}(t) = \prod_r \exp(it\theta_r E_r \otimes B).$$

If $E^2 = E$ then

$$\exp(E \otimes M) = I + \sum_{k\geq 1} \frac{1}{k!} E \otimes M^k = (I - E) \otimes I + E \otimes \exp(M)$$

and accordingly

$$U_{X\times Y}(t) = \prod_r \Big((I - E_r) \otimes I + E_r \otimes U_Y(\theta_r t)\Big).$$

Since $E_r E_s = 0$ if $r \neq s$ and $\prod_r (I - E_r) = 0$, the lemma follows. □

We apply this result to relate uniform mixing on Y and $K_2 \times Y$.

12.6.2 Lemma. *If we have uniform mixing on $K_2 \times Y$, then there is uniform mixing on Y.*

Proof. The eigenvalues of K_2 are 1 and -1 and we denote the corresponding idempotents by E_1 and E_2 respectively. Then by the lemma

$$U_{K_2\times Y}(t) = E_1 \otimes U_Y(t) + E_2 \otimes U_Y(-t)$$

and since

$$E_1 = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}, \qquad E_2 = \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$$

we have

$$U_{K_2\times Y}(t) = \frac{1}{2}\begin{pmatrix}U_Y(t)+U_Y(-t) & U_Y(t)-U_Y(-t)\\ U_Y(t)-U_Y(-t) & U_Y(t)+U_Y(-t)\end{pmatrix}. \qquad (12.6.1)$$

Here the entries of the diagonal blocks are real and those of the off-diagonal blocks are purely imaginary. (You can think about the power series expansions, or use the fact that $K_2 \times X$ is bipartite.)

If $U_{K_2\times Y}(t)$ is flat, we can assume each real entry is of the form $\pm\alpha$ and each complex entry has the form $\pm\alpha i$. This implies that each entry of $U_Y(t)$ is of form $\gamma(\pm 1 \pm i)$, for some γ, and consequently $U_Y(t)$ is flat. □

If we do have uniform mixing on $K_2 \times Y$ at time t, then $U_Y(t) = \gamma H$ where the entries of H are eighth roots of unity. In particular they are algebraic integers. Since

$$1 = \det(U_Y(t)) = \gamma^{|V(Y)|}\det(H)$$

it follows that γ is an algebraic integer too. We will see in Section **??** that this implies that the ratios of the eigenvalues of Y must be rational.

The question of when perfect state transfer occurs on the direct product $X \otimes Y$ is studied by Ge et al. in [30] `http://arxiv.org/pdf/1009.1340v1.pdf` Thus they show that if the eigenvalues of X are odd integers and d is even, then the direct product $X \times Q_d$ admits perfect state transfer. Some of their theory is extended in [21] `http://arxiv.org/abs/1501.04396`

12.7 Double Covers and Switching Graphs

The results in this section come from Coutinho and Godsil [21] `http://arxiv.org/abs/1501.04396`. In particular, Lemma 12.7.2 is Corollary 5.3 in that source.

We begin by introducing a new operation on graphs which includes the products $K_2 \times Y$ as a special case.

If X and Y are graphs with $V(X) = V(Y)$ and with respective adjacency matrices A and B, we define $X \oslash Y$ to be the graph with adjacency matrix

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix}$$

We take $V(X \oslash Y)$ to be $\{0, 1\} \times V(X)$.

One case of interest is when Y is the complement of X, and then we find that $X \oslash \overline{X}$ is the *switching graph* of X. In this case

$$A - B = 2A - I - J,$$

which is usually known as the *Seidel matrix* of X. If X is the empty graph, then $X \oslash Y \cong K_2 \times X$,

We can use this product to construct graphs with perfect state transfer. We see that

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes A + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes B$$

and so if we define

$$H = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

then $H^2 = I$ and

$$(H \otimes I) \begin{pmatrix} A & B \\ B & A \end{pmatrix} (H \otimes I) = \begin{pmatrix} A + B & 0 \\ 0 & A - B \end{pmatrix}.$$

Using this we have

$$(H \otimes I) U_{X \oslash Y}(t) (H \otimes I) = \begin{pmatrix} U_{A+B}(t) & 0 \\ 0 & U_{A-B}(t) \end{pmatrix}$$

and therefore

$$U_{X \oslash Y}(t) = \frac{1}{2} \begin{pmatrix} U_{A+B}(t) + U_{A-B}(t) & U_{A+B}(t) - U_{A-B}(t) \\ U_{A+B}(t) - U_{A-B}(t) & U_{A+B}(t) + U_{A-B}(t) \end{pmatrix}.$$

12.7.1 Theorem. *Let X and Y be graphs with the same vertex set V, and with respective adjacency matrices $A(X)$ and $A(Y)$. The graph $X \oslash Y$ with vertex set $\{0,1\} \times V$ admits perfect state transfer if and only if one of the following holds:*

(a) The matrices $A+B$ and $A-B$ are periodic at time t with respective phase factors λ and $-\lambda$. In this case we get perfect state transfer from $(0,u)$ to $(1,u)$ at time t.

(b) The matrices $A+B$ and $A-B$ admit perfect state transfer from u to v at time t with phase factor λ. We get perfect state transfer at time t between $(0,u)$ and $(0,v)$, and between $(1,u)$ and $(1,v)$.

(c) The matrices $A+B$ and $A-B$ admit perfect state transfer from u to v at time t with respective phase factors λ and $-\lambda$. We get perfect state transfer at time t between $(0,u)$ and $(1,v)$, and between $(1,u)$ and $(0,v)$.

Proof. From our partitioned expression for $U_{X\times Y}(t)$ above, we see that we have pst between $(0,u)$ and $(1,u)$ if and only if

$$|(U_{A+B}(t) - U_{A-B}(t))_{u,u}| = 2.$$

As $|U_{A+B}(t)_{u,u}| \leq 1$ and $|U_{A-B}(t)_{u,u}| \leq 1$, this is equivalent to

$$\lambda = U_{A+B}(t)_{u,u} = -U_{A-B}(t)_{u,u}, \qquad |\lambda| = 1.$$

This proves (a). We see likewise that we have pst from $(0,u)$ to $(0,v)$ if and only if

$$|(U_{A+B}(t) + U_{A-B}(t))_{u,u}| = 2$$

and so (b) follows. Case (c) follows similarly. □

In cases (b) and (c), we see that pst on the factors lifts to pst on $X \oslash Y$. In case (a) we require only periodicity on the factors. We separate out one useful situation. Let $\|x\|_2$ denote the 2-adic norm of the rational number x: if $x = 2^k p/q$ where p and q are odd, then $\|x\|_2 = 2^{-k}$.

12.7.2 Lemma. *Let $\theta_1, \ldots, \theta_d$ be the eigenvalues of the Seidel matrix of X, in non-increasing order and assume $n = |V(X)| > 2$. If $a \in V(X)$, then $X \oslash \overline{X}$ admits perfect state transfer from $(0,a)$ to $(1,a)$ if and only if*

(a) *n is even.*

(b) *The eigenvalue support S of a in X consists of integers.*

(c) *There is a non-negative integer α such that $\|\theta + 1\|_2 = 2^{-\alpha}$ for all θ in S, and $\|n\|_2 = 2^{-\alpha-1}$.*

Proof. We use A and B to denote $A(X)$ and $A(\overline{X})$. Note that $A + B$ is the adjacency matrix of a complete graph K_n, which does not admit pst if $n > 2$. So we are in case (a) of the previous theorem.

We have pst from $(0, a)$ to $(1, a)$ in $X \oslash \overline{X}$ at time t if and only if

$$U_{A+B}(t)_{a,a} = \lambda = -U_{A-B}(t)_{a,a}$$

for some λ with $|\lambda| = 1$. As $A + B = J - I$,

$$U_{A+B}(t) = e^{-it}\left(e^{int}\frac{1}{n}J + \left(I - \frac{1}{n}J\right)\right)$$

and consequently $|U_{A+B}(t)_{a,a}| = 1$ if and only if $t = 2k\pi/n$ for some integer k, and in this case $\lambda = e^{-2ik\pi/n}$.

Now

$$(U_{A-B}(t))_{a,a} = \sum_r e^{it\theta_r}(E_r)_{a,a}$$

and therefore we have pst on $X \oslash \overline{X}$ at time $2k\pi/n$ if and only if

$$-\lambda = e^{2\pi ik\theta_1/n} = \cdots = e^{2\pi ik\theta_d/n}.$$

The lemma follows immediately. □

In a sense, this lemma tells us that if a vertex a in X satisfies a slightly stricter form of our basic periodicity condition, then we have pst in $X \oslash \overline{X}$ from $(0, a)$ to $(1, a)$.

As an example, we note that the eigenvalues of the strongly regular graph $K_n \,\square\, K_n$ are $\{2n-2, n-2, -2\}$. Hence if n is divisible by 4, then the switching graph of $K_n \,\square\, K_n$ admits pst at time $\pi/2$.

12.8 Laplacians and Complements

In [13] (`http://arxiv.org/abs/0808.0748`), Bose et al. considered perfect state transfer on K_n with an edge deleted. They proved that, using the

Laplacian, there is perfect state transfer between the vertices of degree $n-2$ when n is divisible by 4. Here we follow Alvir et al. [2] (`http://arxiv.org/abs/1409.5840`), and derive a more general result.

Let X be a graph on n vertices with adjacency matrix A and diagonal matrix of valencies Δ. Then the corresponding matrices for $\overline{X}$ are $J-I-A$ and $(n-1)I-\Delta$ and therefore

$$L(\overline{X}) = (n-1)I - \Delta - J + I + A = nI - J - L(X).$$

Equivalently

$$L(X) + L(\overline{X}) = L(K_n).$$

Since $AJ = \Delta J$, it follows that L and J commute, and consequently $L(X)$ and $L(\overline{X})$ commute. The eigenvalues of $L(K_n)$ are 0 (with multiplicity 1) and n (with multiplicity $n-1$). Any vector that is constant on the components of X lies in $\ker(L(X))$, and thus 0 is an eigenvalue for $L(X)$ with multiplicity equal to the number of components of X.

12.8.1 Lemma. *Let X be a graph in n vertices. If λ is a non-zero eigenvalue of $L(X)$, then $n-\lambda$ is an eigenvalue of $L(\overline{X})$ with the same multiplicity.* □

12.8.2 Theorem. *Let a and b be vertices in the graph X. If X admits perfect state transfer from a to b at time t relative to the Laplacian and t is an integer multiple of $2\pi/|V(G)|$, then $\overline{X}$ also admits perfect state transfer at time t from a to b.*

Proof. Assume $|V(X)| = n$. We have

$$U_{K_n}(t) = e^{i(n-1)t}\frac{1}{n}J + e^{-it}\left(I - \frac{1}{n}J\right) = e^{-it}\left(e^{in)t}\frac{1}{n}J + \left(I - \frac{1}{n}J\right)\right)$$

and therefore

$$U_{K_n}(2k\pi/n) = e^{-2k\pi i/n}I.$$

Since

$$U_{\overline{X}}(t)U_X(t) = U_{K_n}(t)$$

we see that if we have ab-pst on X at time $2k\pi/n$, then we have ab-pst on $\overline{X}$ at the same time. □

We will see in Lemma 10.7.1 that if perfect state transfer occurs relative to the Laplacian, then the phase factor must be 1. (It might be more rewarding to prove this, rather than look it up.)

If the graph X admits perfect state transfer relative to the Laplacian at time $2k\pi/n$, then so does the graph $X \cup Y$, and does $\overline{X \cup Y}$ (which is the join of the complement of X and Y.)

12.8.3 Corollary. *If Y is a graph and $|V(Y)| \equiv 2$ modulo 4, then the join $\overline{K_2}+Y$ admits perfect state transfer relative to the Laplacian at time $\pi/2$.* □

We conclude that K_n with an edge deleted admits perfect state transfer at time $\pi/2$ between the vertices of degree $n-2$ provided $n \equiv 0$ modulo 4. This is one of the results from Bose et al [13]. The converse to this corollary is proved in Alvir et al [2]: if there is perfect state transfer on the double cone $\overline{K_2}+Y$ at time $\pi/2$, then $|V(Y)| \equiv 2$ modulo 4.

If X is k-regular then $L(X) = kI - A$. Hence we have:

12.8.4 Corollary. *If X is a k-regular graph on n vertices that admits perfect state transfer relative to the adjacency matrix between vertices a and b at time an integer multiple of $2\pi/n$, then $\overline{X}$ admits perfect state transfer relative to the adjacency matrix between a and b at the same time.* □

Notes

Although the constructions presented in this chapter are simple, together they give all examples of pst on graphs with at most nine vertices. The only other examples of pst come from distance-regular graphs (see Section 14.9), or from Cayley graphs for abelian groups (Chapter 16).

Exercises

Part IV

Algebraic Connections

Chapter 13

Orthogonal Polynomials

Let $\mathrm{Pol}(n)$ be the vector space of all real polynomials of degree at most n, and let Pol denote the vector space of all real polynomials. These vector spaces come with many possible inner products, for example,

$$\langle p, q\rangle = \int_0^\infty p(x)q(x)\, e^{-x} dx.$$

Once we have chosen an inner product, we use Gram-Schmidt to derive an orthogonal basis from the basis

$$1,\ x,\ x^2, \dots,$$

and hence we arrive at a sequence of polynomials

$$p_0,\ p_1,\ p_2, \dots$$

where p_r has degree r and $\langle p_r, p_s\rangle = 0$ if $r \neq s$. We call such a sequence of *orthogonal polynomials*. Note that the sequence is not unique, we can replace each p_r by a non-zero scalar multiple and the result is still a sequence of orthogonal polynomials. There are a number of standard ways to normalize the sequence. We might arrange that for all r:

(a) $\langle p_r, p_r\rangle = 1$.

(b) $p_r(a) = 1$ for some suitable real number a.

(c) p_r is monic.

For us, the third choice will be most common.

We impose one restriction on the inner product we use: for any polynomials p and q we must have

$$\langle xp, q\rangle = \langle p, xq\rangle.$$

(In other terms, multiplication by x must be a self-adjoint operator.)

13.1 Examples

We discuss two of the cases where orthogonal polynomials arise in combinatorics.

Matching Polynomials

The first is in the theory of matching polynomials. If X is a graph on n vertices, let $p(X,k)$ denote the number of k matchings in X and define the *matching polynomial* $\mu(X,t)$ by

$$\mu(X,t) = \sum_{k\geq 0} (-1)^k p(X,k) t^{n-2k}.$$

This can viewed as a modified form of generating function for the matchings in X, weighted by their size. One effect of the modifications is that if X is a forest then its matching and characteristic polynomials coincide.

Our next result is a somewhat surprising property of the matching polynomial. (This comes from [34].)

13.1.1 Theorem. *The number of perfect matchings in the complement of the graph X is equal to*

$$\frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} \mu(X,t)\, e^{-t^2/2} dt.$$ □

Since

$$\mu(K_m \cup K_n, t) = \mu(K_m, t)\mu(K_n, t)$$

and since $\overline{K_m \cup K_n}$ is the complete bipartite graph $K_{m,n}$, it follows from this theorem that the polynomials $\mu(K_r, t)$ are the orthogonal polynomials relative to the inner product

$$\langle p, q\rangle = \frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} p(t)q(t)\, e^{-t^2/2} dt.$$

They are the *Hermite polynomials*. Using similar ideas it can be shown that, for each non-negative integer a, the sequence

$$\mu(K_{m,m+a}, t), \quad m = 0, 1, \dots$$

is a family of orthogonal polynomials. (They are *Laguerre polynomials*.)

The sequences $(\mu(P_r, t))_{r\geq 0}$ and $(\mu(C_r, t))_{r\geq 0}$ are orthogonal polynomials, corresponding to the two types of *Chebyshev polynomials*. (I do not know a nice combinatorial proof that these polynomials are orthogonal.)

Distance-Regular Graphs

Let X be a graph with exactly $d+1$ distinct eigenvalues $\theta_0, \dots, \theta_d$ and with adjacency matrix A. Define an inner product on polynomials by

$$\langle p, q\rangle := \operatorname{tr}(p(A)q(A)).$$

Is this an inner product? It is certainly bilinear and symmetric and

$$\langle p, p\rangle \geq 0$$

for any polynomial p. But if $p(A) = 0$ then $\langle p, p\rangle = 0$ and therefore $\langle p, p\rangle = 0$ does not imply that $p = 0$. There are two ways to deal with this. Once is to confine ourselves to the polynomials of degree at most d. The second, and preferable, approach is to declare that we are working with "polynomials restricted to the spectrum of A". Thus our objects are now equivalence classes of polynomials—two polynomials are equivalent if they agree on each eigenvalue of A—and each equivalence class contains a unique polynomial of degree at most d. If $E_0, \dots, E_d$ are the idempotents in the spectral decomposition of A then $E_r = f_r(A)$ for some polynomial f_r of degree at most d and therefore when $r \neq s$,

$$\langle f_r, f_s\rangle = \operatorname{tr}(E_r E_s) = 0.$$

However the polynomials f_r do not form a sequence of orthogonal polynomials because they do not satisfy the degree constraint.

So using Gram-Schmidt on the polynomials

$$1, x, x^2, \dots, x^d$$

we construct a sequence of orthogonal polynomials

$$p_0, p_1, \ldots, p_d.$$

If we take these to be monic, then $p_0 = 1$ and $p_1(x) = x$. Let $\operatorname{sum}(M)$ denote the sum of the entries of the matrix M. Then for symmetric matrices

$$\operatorname{tr}(MN) = \operatorname{sum}(M \circ N).$$

If $r \neq s$ we have

$$\langle p_r, p_s \rangle = \operatorname{tr}(p_r(A)p_s(A)) = \operatorname{sum}(p_r(A) \circ p_s(A)).$$

Now suppose X has diameter d and that its distance matrices are $A_0, \ldots, A_d$. Then if $r \neq s$

$$\operatorname{tr} A_r A_s = \operatorname{sum}(A_r \circ A_s) = 0.$$

In general A_r is not a polynomial of degree r in A_1, but if X is distance-regular then there are polynomials $p_0, \ldots, p_d$ such that $\deg(p_r) = r$ and $A_r = p_r(A_1)$. Hence this sequence of polynomials is the sequence of orthogonal polynomials relative to our inner product. In these setting it can be useful to define p_{d+1} to be the minimal polynomial of A_1; it is the zero polynomial of degree $d+1$ on the spectrum of A_1.

13.2 The Three-Term Recurrence

Suppose we have a sequence of orthogonal polynomial relative to an inner product. Our first observation is simple but important:

13.2.1 Lemma. *If $(p_r)_{r \geq 0}$ is a sequence of orthogonal polynomials then p_r is the unique (up to multiplication by a non-zero scalar) polynomial of degree r that is orthogonal to all polynomials of degree less than r.* □

Equivalently if q_r is the orthogonal projection of t^r on the space of polynomials of degree less than r, then p_r is a scalar multiple of $t^r - q_r$.

Now

$$\langle tp_r, p_s \rangle = \langle p_r, tp_s \rangle,$$

whence we see that $\langle tp_r, p_s\rangle = 0$ unless $|r-s| \le 1$. Consequently there are scalars α_r, β_r, γ_r such that

$$tp_r = \gamma_r p_{r+1} + \alpha_r p_r + \beta_r p_{r-1}. \tag{13.2.1}$$

We can be more specific:

13.2.2 Theorem. *If $(p_r)_{r\ge 0}$ is a sequence of monic orthogonal polynomials, then*

$$p_{r+1} = (t-a_r)p_r - b_r p_{r-1}. \tag{13.2.2}$$

where

$$a_r = \frac{\langle tp_r, p_r\rangle}{\langle p_r, p_r\rangle}, \qquad b_r = \frac{\langle p_r, p_r\rangle}{\langle p_{r-1}, p_{r-1}\rangle} \tag{13.2.3}$$

Proof. If our polynomials are monic then γ_r in (13.2.1) is 1 and

$$\langle tp_r, p_r\rangle = \alpha_r \langle p_r, p_r\rangle$$

which yields the expression for a_r. Next

$$\langle tp_r, p_{r-1}\rangle = \beta_r \langle p_{r-1}, p_{r-1}\rangle$$

and since our polynomials are monic

$$\langle tp_r, p_{r-1}\rangle = \langle p_r, tp_{r-1}\rangle = \langle p_r, p_r\rangle$$

from which our formula for b_r follows. □

Clearly we can use the three-term recurrence to compute expressions for the members of a sequence of orthogonal polynomials, starting with p_0 and p_1. It is worth noting that we can run the recurrence in reverse: given p_d and p_{d-1}, we can compute all the initial terms in the sequence. In fact we do not need the coefficients a_i and b_i, for there is a unique α such that

$$p_d(t) - (t-\alpha)p_{d-1}(t)$$

has degree $d-2$, and if β is the coefficient of x^{d-2} in this difference, then

$$p_{d-2}(t) = \frac{1}{\beta}(p_d(t) - (t-\alpha)p_{d-1}(t)).$$

Continuing in this way, we can reconstruct all the polynomials $p_0, \ldots, p_{d-2}$.

13.3 Tridiagonal Matrices

A matrix T is *tridiagonal* if $T_{i,j} = 0$ whenever $|i-j| > 1$. It is *irreducible* if $T_{i+1,i}T_{i,i+1} \neq 0$ for all i. We will assume without comment that our tridiagonal matrices are irreducible; we also assume that the off-diagonal entries $T_{i,i+1}$ and $T_{i+1,i}$ are non-negative, for all i. (Although all that is really needed is that the products $T_{i+1,i}T_{i,i+1}$ be non-negative.) We can view an irreducible tridiagonal matrix as a weighted adjacency matrix for a matrix, and this viewpoint is useful as well as natural. The index sets for the rows and columns of a matrix will start at 0.

A tridiagonal matrix T of order $d \times d$ determines a sequence of monic polynomials $p_0, \ldots, p_d$, where $p_0 = 1$ and p_r is the characteristic polynomial of the leading principal $r \times r$ submatrix of T. We call these polynomials the *polynomial sequence* associated with T. We will see that any such sequence is a finite sequence of orthogonal polynomial.

13.3.1 Lemma. *If T is the tridiagonal matrix*

$$T := \begin{pmatrix} a_0 & 1 & & & \\ b_1 & a_1 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{d-2} & a_{d-2} & 1 \\ & & & b_{d-1} & a_{d-1} \end{pmatrix}$$

and $p_0, \ldots, p_d$ is the associated sequence of orthogonal polynomials, then these polynomials satisfy the recurrence

$$p_{r+1} = (t - a_r)p_r - b_r p_{r-1}.$$

Proof. We leave this to the reader. □

There is another, more high-flown, way to view this. The ring $\mathbb{R}[t]/(p_d(t))$ is a vector space over $\mathbb{R}$. Multiplication by t is a linear map on this vector space, and T is the matrix that represents this map, relative to the basis $p_0, \ldots, p_{d-1}$.

If T is tridiagonal and D is a diagonal matrix of the same order as T with positive diagonal entries, then $D^{-1}TD$ is tridiagonal. The sequence of polynomials associated with $D^{-1}TD$ is the same as that associated with T because the sequence belonging to a tridiagonal matrix T is determined by the products $T_{i+1,i}T_{i,i+1}$. If S and T are tridiagonal of the same order then

$$S_{i+1,i}S_{i,i+1} = T_{i+1,i}T_{i,i+1}$$

for all i if and only if there is a diagonal matrix D with positive diagonal entries such that $S = D^{-1}TS$. For future reference we spell out an important special case of this.

13.3.2 Lemma. *Let T be a tridiagonal matrix of order $d \times d$, with $T_{r,r+1} = 1$ for all r. Let B be the $d \times d$ diagonal matrix with $B_{0,0} = 1$ and $B_{r,r} = \prod_{j=1}^{r} b_j$ when $r > 0$. Then*

$$B^{-1/2}TB^{1/2} = \begin{pmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{b_{d-2}} & a_{d-2} & \sqrt{b_{d-1}} \\ & & & \sqrt{b_{d-1}} & a_{d-1} \end{pmatrix}. \qquad \square$$

Referring back to Theorem 13.2.2, we see that

$$B_{r,r} = \langle p_r, p_r \rangle.$$

An immediate consequence of the previous lemma is that the eigenvalues of a tridiagonal matrix are real. Rather more is true:

13.3.3 Theorem. *If $(p_r)_{r \geq 0}$ is a sequence of orthogonal polynomials, then the zeros of each polynomial are real and simple. Further the zeros of p_{r+1} are interlaced by those of p_r.* □

Proof. The eigenvalues are real as just noted. The interlacing is the usual interlacing of eigenvalues for weighted graphs. This leaves simplicity. If T is tridiagonal of order $d \times d$ then the matrix we get from $T - \lambda I$ by deleting the first row and last column is upper triangular with positive diagonal entries, and hence its rank is $d - 1$. Consequently the rank of $T - \lambda I$ is at least $d - 1$, for any λ, and therefore the eigenvalues of T are simple. □

13.4 Eigenvectors

We show that the polynomials $p_0, \dots, p_{d-1}$ associated with a tridiagonal matrix are orthogonal with respect to an inner product.

Assume T is tridiagonal of order $d \times d$ and $T_{i+1,i} = 1$ for all i. The reader might verify that

$$T \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{d-1} \end{pmatrix} = t \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{d-1} \end{pmatrix} - p_d(t) \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

and therefore, if θ is an eigenvalue of T,

$$\tilde{p}(\theta) := \begin{pmatrix} p_0(\theta) \\ p_1(\theta) \\ \vdots \\ p_{d-1}(\theta) \end{pmatrix}$$

is an eigenvector for T with eigenvalue θ.

So $B^{-1/2}\tilde{p}(\theta)$ is an eigenvector for the symmetric matrix $B^{-1/2}B^{1/2}$, and therefore if θ_i and θ_j are distinct zeros of p_{d+1}, the vectors

$$B^{-1/2}\tilde{p}(\theta_i), \quad B^{-1/2}\tilde{p}(\theta_j)$$

must be orthogonal (with respect to the usual inner product on $\mathbb{R}^{d+1}$). Therefore the columns of the matrix

$$B^{-1/2}\begin{pmatrix} \tilde{p}(\theta_0) & \dots & \tilde{p}(\theta_d) \end{pmatrix}$$

are pairwise orthogonal. We set

$$\beta_i = B_{i,i},$$

and then the squared norm of the r-th column of our matrix of eigenvectors is

$$\nu_r := \sum_i \frac{p_i(\theta_r)^2}{\beta_i}.$$

If we multiply the r-th column by ν_r^{-1}, for each r, then the rows of the resulting matrix are orthogonal too, which implies that if $i \neq j$, then

$$\sum_{r=0}^{d-1} \nu_r^{-1} p_i(\theta_r) p_j(\theta_r) = 0.$$

We now define

$$\langle p_i, p_j \rangle := \sum_{r=0}^{d-1} \nu_r^{-1} p_i(\theta_r) p_j(\theta_r),$$

and thus we have an inner product on the space of polynomials of degree at most d, relative to which the sequence $(p_r)_{r=0}^d$ is orthogonal.

Note that if we have an infinite sequence of orthogonal polynomials, then we have an infinite sequence of inner products. Under reasonable conditions this sequence will converge to a limit. This is known as *Favard's Theorem*.

13.5 Orthogonality

Let A be a symmetric matrix of order $d \times d$. We define a family of inner products on the algebra of real polynomials in one variable. Let M be a positive semidefinite matrix of order $d \times d$ and set

$$[p, q] := \operatorname{tr}(p(A)q(A)M).$$

This is a symmetric bilinear function and, since $M \succcurlyeq 0$ we have

$$[p, p] = \operatorname{tr}(p(A)^2 M) \geq 0.$$

However, we need to know when $[p, p] > 0$. Note that if p and q are polynomials such that $p(A)M = q(A)M = 0$ and f and g are polynomials, then

$$(f(A)p(A) + g(A)q(A))M = 0.$$

It follows that there is a unique monic polynomial ψ_M of least degree such that if $f(A)M = 0$, then ψ_M divides f. (In particular, ψ_M divides the minimal polynomial of A.)

Let T be a tridiagonal matrix of order $d \times d$. Let $p_r(t)$ be the characteristic polynomial of the leading $r \times r$ submatrix of T and set $p_0(t) = 1$. We prove that the polynomials $p_0, \ldots, p_d$ are orthogonal.

13.5.1 Lemma. *If $M \succcurlyeq 0$ and A is symmetric, the bilinear map*

$$[p, q] = \operatorname{tr}(p(A)q(A)M)$$

is an inner product on the space of polynomials with degree less than $\deg(\psi_M)$.

Proof. Since $M \succcurlyeq 0$, it has a positive semidefinite square root $M^{1/2}$. Now

$$\text{tr}(p(A)^2 M) = \text{tr}(M^{1/2} p(A)^2 M^{1/2}),$$

since $\text{tr}(B^T B) = 0$ if and only if $B = 0$ we have that $[p,p] = 0$ if and only if $p(A)M^{1/2} = 0$, and this holds if and only $p(A)M = 0$. (Note that $M^{1/2}$ and M have the same column space.) □

We have already made use of an inner product of this form in Subsection 13.1, with $M = I$.

There is one important case where inner products of the above form arise naturally. Suppose A is symmetric matrix and x is a vector such that the cyclic A-module $\langle x \rangle_A$ it generates has dimension d. Then the vectors

$$x,\ Ax, \ldots, A^{d-1}x$$

are linearly independent, and therefore they are a basis for $\langle x \rangle_A$. We can apply the Gram-Schmidt algorithm to these vectors to produce an orthogonal basis $y_0, \ldots, y_{d_1}$ for $\langle x \rangle_A$, and it is an easy exercise to see that there are polynomials $p_0, \ldots, p_{d-1}$ such that $\deg(p_r) = r$ and $y_r = p_r(A)x$. Hence

$$x^T p_r(A) p_s(A) x = 0$$

if $r \neq s$ and so our polynomials are orthogonal relative to the inner product

$$[p,q] = \text{tr}(p(A)q(A)xx^T).$$

Finally we note that the matrix B that represents the action of A on $\langle x \rangle_A$ is tridiagonal. It follows that any algorithm for determining the eigenvalues of a tridiagonal matrix can be used to get the eigenvalues of a symmetric matrix. The standard QR-algorithm for computing the eigenvalues of symmetric matrices does first convert the input to tridiagonal form (although it does not use Gram-Schmidt to do this).

13.6 A Trace Inner Product for Orthogonal Polynomials

13.6.1 Lemma. *Let T be a tridiagonal matrix of order $d \times d$ with associated polynomials $p_0, \ldots, p_d$ and set $\beta_r = \prod_{i=1}^r b_r$. Then*

$$p_r(T)e_0 = \beta_r e_r.$$

Proof. We proceed by induction on r. The result is trivial when $r = 0$; for $r = 1$ we have $p_1(t) = t - a_1$ and hence

$$p_1(T)e_0 = (T - a_1 I)e_0 = b_1 e_1 = \beta_1 e_1.$$

Assume $r \geq 1$. Then

$$Te_r = e_{r-1} + a_r e_r + b_{r+1} e_{r+1}$$

and

$$\begin{aligned} p_{r+1}(T)e_0 &= (T - a_r I)p_r(T)e_0 - b_r p_{r-1}(T)e_0 \\ &= \beta_r (T - a_r I)e_r - b_r \beta_{r-1} e_{r-1} \\ &= \beta_r b_{r+1} e_{r+1} + (\beta_r - b_r \beta_{r-1})e_r \\ &= \beta_{r+1} e_{r+1}. \end{aligned}$$

□

Assume T is tridiagonal of order $d \times d$ and

$$\hat{T} = B^{-1/2} T B^{1/2},$$

as in Lemma 13.3.2. If you completed the exercise assigned there, you know that $B_{r,r} = \beta_r$. (We assume $\beta_0 = 1$.) We have

$$p_r(\hat{T})e_0 = B^{-1/2} p_r(T) B^{1/2} e_0 = B^{-1/2} p_r(T) e_0 = \beta_r B^{-1/2} e_r = \beta_r^{1/2} e_r,$$

and consequently

$$\langle p_r(\hat{T})e_0, p_s(\hat{T})e_0 \rangle = \beta_r \delta_{r,s}.$$

13.6.2 Theorem. *Let T be a tridiagonal matrix of order $d \times d$ and let $p_0, \dots, p_d$ be the family of monic polynomials associated to T. Then these polynomials are orthogonal relative to the inner product on polynomials of degree at most $d - 1$ given by*

$$[f, g] = \operatorname{tr}(f(\hat{T}) g(\hat{T}) e_0 e_0^T).$$

□

If we have the spectral decomposition

$$\hat{T} = \sum_r \theta_r E_r,$$

then

$$[f, g] = \sum_r f(\theta_r) g(\theta_r) \operatorname{tr}(E_r e_0 e_0^T) = \sum_r f(\theta_r) g(\theta_r) (E_r)_{0,0}.$$

To make this useful, in the following section we determine $(E_r)_{0,0}$.

13.7 Spectral Idempotents

Let T be a tridiagonal matrix with $T_{r,r+1} = 1$ for all r, and let $\hat{T}$ be the symmetrized version of T. We determine the spectral idempotents of $\hat{T}$.

Let $p_0, \dots, p_d$ be the sequence of monic polynomials associated with T and let B be the diagonal matrix such that $B^{-1/2}TB^{1/2} = \hat{T}$. If θ_r is an eigenvalue of T, the vector $\tilde{p}_r$ with i-th entry $\beta_i^{-1/2} p_i(\theta_r)$ is an eigenvector for $\hat{T}$. Let ν_r denote the squared norm of this vector. As the eigenvalues of $\hat{T}$ are simple, this implies that the idempotent E_r associated with θ_r is equal to $\nu_r^{-1} \tilde{p}_r t p_r^T$. Hence

$$(E_r)_{0,0} = \frac{1}{\nu_r}$$

and our only problem is to determine ν_r.

If we use p_d to denote $\det(tI - T)$ then, by Equation (4.3.4), we have

$$(E_r)_{d-1,d-1} = \frac{p_{d-1}(\theta_r)}{p_d'(\theta_r)}$$

and since we also have

$$(E_r)_{d-1,d-1} = \frac{p_{d-1}(\theta_r)^2}{\beta_{d-1}\nu_r},$$

it follows that

$$\nu_r = \frac{p_{d-1}(\theta_r) p_d'(\theta_r)}{\beta_{d-1}}.$$

We recall that $\beta_r = \langle p_r, p_r \rangle$.

13.8 Interlacing

Suppose p and q are polynomials of degree $n-1$ and n respectively and the zeros of q are

$$\zeta_1, \dots, \zeta_n.$$

We say that p *interlaces* q if the zeros of q are real and for $r = 1, \dots, n-1$ each interval $[\zeta_r, \zeta_{r+1}]$ contains a zero of p.

The canonical example arises when $q = p'$. If $\theta_1, \dots, \theta_n$ are the zeros of p in decreasing order and m_r denotes the multiplicity of θ_r as a zero of p, then

$$\frac{p'(t)}{p(t)} = \sum_r \frac{m_r}{t - \theta_r}.$$

The derivative of $p'(t)/p(t)$ is negative wherever it is defined. Since p'/p is continuous on each open interval (θ_r, θ_r+1) and since it changes sign on this interval, there is a zero of p' in (θ_r, θ_r+1). Therefore p' interlaces p.

13.8.1 Lemma. *If q and p are monic polynomials of degree $n-1$ and n respectively. Then the following are equivalent:*

(a) q interlaces p.

(b) The poles of the rational function $q(t)/p(t)$ are real and simple, and the residue at each pole is positive.

(c) If t is not a zero of p then $(q(t)/p(t))' < 0$.

(d) If t is not a zero of q then $(p(t)/q(t))' \geq 1$.

Proof. There is no loss in assuming that q and p are coprime. Let $\theta_1, \dots, \theta_n$ be the zeros of p in decreasing order. We consider the the rational function q/p. Since the zeros of p are simple, each pole of q/p is simple and we have a partial fraction expansion

$$\frac{q(t)}{p(t)} = \sum_r \frac{c_r}{t-\theta_r}$$

for some nonzero constants c_r. A simple limit computation yields that $c_r = q(\theta_r)/p'(\theta_r)$ and, since the sign of both $p'(\theta_r)$ and $q(\theta_r)$ is $(-1)^{r-1}$ we conclude that $c_r > 0$.

If $c_r > 0$ for each r then $(q/p)'$ is negative wherever it is defined and so (b) implies (c). It is easy to see that the converse is true. □

As an application, we sketch a proof that the zeros of the path P_n are real. We use induction on n with a stronger claim: we assume that if $k < n$ then the zeros of P_k are real and $\phi_{k-1}(t)$ interlaces $\phi_k(t)$. Now using the recurrence for $\phi_n(t)$, we have

$$\frac{\phi_n(t)}{\phi_{n-1}(t)} = t - \frac{\phi_{n-1}(t)}{\phi_n(t)}.$$

Suppose the right side has exactly m poles. By looking at its graph, we see that it has $m+1$ distinct zeros. Hence the reciprocal of the left side has exactly $m+1$ poles, since the derivative of the right side is positive wherever it's defined it follows that $\phi_{n-1}(t)/\phi_n(t)$ has $m+1$ poles, all real, and since the zeros of $\phi_{n-1}(t)$ are real we conclude that all zeros $\phi_n(t)$ are real.

13.9 Sturm Sequences

A sequence of polynomials $p_0, \dots, p_m$ is a *Sturm sequence* if $\deg(p_r) = r$, the leading term of each polynomial is positive, and consecutive terms interlace. We note:

13.9.1 Lemma. *Suppose p and q are monic polynomials of degree n and $n-1$, where $n \geq 2$. If q interlaces p, then there are scalars a and b and a monic polynomial r such that $b > 0$ and*

$$p(t) = (t-a)q(t) - br(t).$$

Furthermore r interlaces q. □

Proof. First we note that

$$\frac{p}{q} = t - a - b\frac{r}{q}$$

whence

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

If we can show that $(p/q)' > 1$, then $b(q/p)' < 0$. Since $(r/q)'$ is negative when t is large it follows that $b > 0$ and $(r/q)' < 0$ and therefore r interlaces q.

We have

$$q^2\left(\frac{p}{q}\right)' = p'q - pq' = -p^2\left(\frac{q}{p}\right)' \tag{13.9.1}$$

Next

$$p^2\left(\frac{q}{p}\right)' = -\sum_r c_r \frac{p(t)^2}{(t-\theta_r)^2}$$

and

$$q^2 = \left(\sum_r c_r \frac{p(t)}{t-\theta_r}\right)^2$$

and so from (13.9.1) we have

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

Since p and q are monic, $\sum_r c_r = 1$ and therefore

$$\left(\sum_r c_r \frac{p(t)}{t-\theta_r}\right) \leq \sum_r c_r \frac{p(t)^2}{(t-\theta_r)^2};$$

it follows that $(p/q)' \geq 1$. The inequality is strict unless there is only one term in the sum, in which case $n = 1$. □

The previous lemma yields the following by induction.

13.9.2 Lemma. *The sequence of monic polynomials $p_0, \ldots, p_n$ is a Sturm sequence if and only there are real numbers a_r and b_r for $r = 1, \ldots, n$ such that $b_r > 0$*

$$p_{r+1} = (t - a_r)p_r - b_r p_{r-1}. \qquad \square$$

Our next result follows from, for example, [41, Theorem 6.3a].

13.9.3 Theorem. *Suppose $p(t)$ is a polynomial of degree n with real distinct zeros and let $q_0, \ldots, q_n$ be a Sturm sequence with $q_n = p$. Let $\zeta_1, \ldots, \zeta_n$ be the zeros of p in decreasing order. Then there are at most $r-1$ zeros and exactly $r-1$ sign changes in the sequence*

$$(q_0(\zeta_r), q_1(\zeta_r), \ldots, q_{n-1}(\zeta_r)). \qquad \square$$

In counting the sign changes in a sequence, we first delete all zeros from the sequence. (If there is a zero at an internal term of the original sequence, the terms that bracket it will have opposite sign.)

13.10 Balanced Paths

If a weighted path admits perfect state transfer between its end-vertices at time t, then the end-vertices must be strongly cospectral. (Recall that for graphs with only simple eigenvalues, cospectral vertices are automatically strongly cospectral.) Let P be a weighted path with vertex set $\{0, \ldots, d-1\}$; we say that P is *balanced* if the permutation that sends i to $d-1-i$ (for each i) is an automorphism.

13.10.1 Lemma. *Let P be a weighted path of length d, with vertex set $\{0, \ldots, d-1\}$. and let $E_0, \ldots, E_{d-1}$ be the spectral idempotents for $A(P)$. If the end-vertices of P are cospectral, then P is symmetric. Further if R is the automorphism that swaps the end-vertices of P, then R is a polynomial in $A(P)$ and $R = \sum_{k=0}^{d-1} (-1)^k E_k$.*

Proof. If the end-vertices of P are strongly cospectral, then by Lemma 6.8.1, there is an orthogonal matrix R which is a polynomial in A and swaps e_0 and e_{d-1}. Hence

$$A^j e_{d-1} = A^j Re_0 = RA^j e_0$$

and it follows, after some effort on the reader's part, that $Re_j = e_{d-1-j}$. Therefore R is an automorphism of P.

Suppose z is an eigenvector for A. Then it is an eigenvector for R (because R is a polynomial in A) and, since $R^2 = I$, it follows that $Rz = \pm z$. If $p_0, \ldots, p_{d-1}$ is the sequence of polynomials associated with A, then we may assume that $z_i = \beta_i^{-1/2} p_i(\theta_k)$, for some eigenvalue θ_k. We see that $z_0 = 1$ and the sign of z_{d-1} is equal to the sign of $p_{d-1}(\theta_k)$, and thus it is $(-1)^k$. Consequently if z belongs to the eigenvalue θ_k, then $Rz = (-1)^k z$. As the idempotent belonging to θ_k is a scalar multiple of zz^T, we deduce that $RE_k = (-1)^k E_k$ and therefore the spectral decomposition of R is as stated. □

13.10.2 Corollary. *Let P be a weighted path on d vertices with adjacency matrix A. Then P is balanced if and only if $p_{d-1}(A) = \gamma R$ for some γ.*

Proof. Assume that P is balanced. By Lemma 13.6.1, we have $p_{d-1}(A)e_0 = \beta_{d-1}e_{d-1}$ and, since $Re_{d-1} = e_0$, it follows that $Rp_{d-1}(A)e_0 = \beta_{d-1}e_0$. As R and $p_{d-1}(A)$ commute with A, it follows that

$$Rp_{d-1}(A)e_0 A^k = \beta_{d-1} A^k e_0$$

for all k and therefore $Rp_{d-1}(A) = \beta_{d-1} I$.

Now suppose that $p_{d-1}(A) = \gamma R$ for some γ. The sequence of polynomials $p_0, \ldots, p_d$ can be constructed by running the three-term recurrence backwards from p_d and p_{d-1}. Since R commutes with $p_d(A)$ (which is zero) and with $p_{d-1}(A)$, it follows that R commutes with $p_1(A) = A - a_0 I$. Therefore R commutes with A and so P is balanced. □

Note that it is easy to constructed weighted paths with given spectrum. Suppose we are given distinct reals

$$\theta_0 > \theta_1 > \cdots > \theta_{d-1}.$$

Define $p_d(t) = \prod_i (t - \theta_i)$, let ℓ_i denote the Lagrange interpolating polynomial

$$\ell_i(t) = \prod_{j:j \neq i} \frac{t - \theta_j}{\theta_i - \theta_j}$$

and let $a_0, \dots, a_{d-1}$ be a sequence of positive reals. Define

$$p_{d-1}(t) := \sum_{i=0}^{d-1} (-1)^i a_i \ell_i(t).$$

Then p_{d-1} interlaces p_d and so, using the Euclidean algorithm we can construct a sequence of polynomials $p_0, \dots, p_d$. The eigenvalues of the associated tridiagonal matrix are the given reals $\theta_0, \dots, \theta_{d-1}$.

Furthermore, if in this construction, we take $a_i = 1$ for all i, then p_{d-1} is a scalar multiple of R, and the path we construct will be balanced.

13.11 Designer Transfers

We present a method for constructing weighted paths with perfect state transfer between their end-vertices. The basic idea is to construct the path from its eigenvalues.

If A is the adjacency matrix of a weighted path and c and d are real numbers (with $d > 0$), then $cI + dA$ is the adjacency matrix of a weighted path, and we have pst relative to A if and only we have pst relative to $cI + dA$. We say that the second path is obtained from the first by *shifting and scaling*. If we have pst on P, we have pst on any weighted path obtained from it by shifting and (non-zero) scaling.

13.11.1 Lemma. *Let P be a weighted path on d vertices with eigenvalues $\theta_1, \dots, \theta_d$. If there is perfect state transfer between the end-vertices of P, then there is a shifting and scaling of P with all eigenvalues integers.*

Proof. Our argument is, at most, a simple variant of the the one we used to prove Theorem 7.6.1. There we assumed that the entries of A were integers.

Let A denote the adjacency matrix of P and set $U(t) = \exp(itA)$. Then

$$U(t)_{a,b} = \sum_r e^{it\theta_r} (E_r)_{a,b}$$

and therefore, by the triangle inequality,

$$|U(t)_{a,b}| \leq \sum_r |(E_r)_{a,b}|.$$

Equality holds if and only if there is a complex scalar γ such that

$$e^{it\theta_r} \operatorname{sign}((E_r)_{a,b}) = \gamma$$

for all r. As in the proof of Theorem 7.6.1, we conclude that if there is ab-pst on P, then the ratio condition holds:

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_\ell} \in \mathbb{Q}$$

for all r, s, k, ℓ with $k \neq \ell$.

It follows that for some rational number C we have

$$C \prod_{r \neq s} (\theta_r - \theta_s) = (\theta_1 - \theta_2)^{(d-1)(d-2)}.$$

We assume now that P is scaled so that the product on the left is an integer. Since θ_1 and θ_2 are real, we infer that $(\theta_1 - \theta_2)^2$ is rational, and consequently we can assume that P is scaled so that the eigenvalue differences are integers. Now we can shift P so that the eigenvalues themselves are integers. □

13.11.2 Theorem. *Let $\theta_0, \ldots, \theta_{d-1}$ be a strictly decreasing series of integers. Then there is a unique weighted path P on d vertices with eigenvalues $\theta_0, \ldots, \theta_{d-1}$ and with perfect state transfer between its end-vertices.*

Proof. Set

$$p_d(t) = \prod_{r=0}^{d-1} (t - \theta_r)$$

and let f be the unique polynomial of degree $d-1$ such that

$$f(\theta_r) = (-1)^r.$$

If f_0 is the leading term of f, set $p_{d-1}(t) = f_0^{-1} f(t)$.

Let $p_0, \ldots, p_{d-1}$ be the sequence of orthogonal polynomials constructed from p_{d-1} and p_d, let A be the associated symmetric tridiagonal matrix and let P the weighted path with adjacency matrix A. Then P has perfect state transfer between its end vertices. □

The path just constructed will have no loops if and only if the eigenvalues are symmetric about the origin.

13.12 Unbalanced Paths with Perfect State Transfer

We present a construction due to Kay [45] of unbalanced paths on five vertices that admit pst between the second and fourth vertices, but not between the end-vertices.

We consider the weighted path P of length five with symmetric adjacency matrix

$$\begin{pmatrix} 0 & \sqrt{a} & 0 & 0 & 0 \\ \sqrt{a} & 0 & \sqrt{b} & 0 & 0 \\ 0 & \sqrt{b} & 0 & \sqrt{c} & 0 \\ 0 & 0 & \sqrt{c} & 0 & \sqrt{d} \\ 0 & 0 & 0 & \sqrt{d} & 0 \end{pmatrix}.$$

The characteristic polynomial of this matrix is

$$t^5 - (a+b+c+d)t^3 + (ac+ad+bd)t = t((t^2-a-b)(t^2-c-d)-bc).$$

The respective characteristic polynomials of $T\setminus 2$ and $T\setminus 4$ are

$$t^2(t^2-c-d), \quad t^2(t^2-a-b)$$

whence the vertices 2 and 4 are strongly cospectral if and only if

$$a+b=c+d.$$

In this case the eigenvalues of P are

$$0,\ \pm\sqrt{a+b\pm\sqrt{bc}}.$$

Note that the eigenvalue support of 2 (and of 4) consists of the four non-zero eigenvalues of P. The characteristic polynomials of $T\setminus 1$ and $T\setminus 2$ respectively are

$$t^4-(a+b+c)t^2+ac, \qquad t^4-(b+c+d)t^2+bd;$$

these are equal only if $a=d$ and $b=c$, that is, if and only if P is balanced.

Following Kay, we assume $a+b=c+d$ and take

$$a+b=\frac{5}{2}, \quad bc=3/2.$$

The characteristic polynomial of P is then

$$t((t^2-5/2)^2-3/2)=t(t^4-5t^2+4)=t(t^2-1)(t^2-4)$$

and so the eigenvalues of P are

$$-2,\ -1,\ 0,\ 1,\ 2.$$

Some calculation yields that

$$U(\pi)=\frac{1}{16}\begin{pmatrix}4&0&6&0&6\\0&0&0&16&0\\6&0&9&0&1\\0&16&0&0&0\\6&0&1&0&9\end{pmatrix}$$

and so we have pst from 2 to 4 at time π.

Note that we may take $a=0$, when we get pst on a weighted path with four vertices, from vertex 1 to vertex 3.

Notes

Exercises

Chapter 14

Association Schemes

This chapter provides an introduction to some aspects of association schemes and related algebras. We use the machinery we develop to construct new examples of graphs with perfect state transfer. In later chapters we will find further applications of the theory, in particular when we discuss uniform mixing.

14.1 Automorphisms and Algebras

The definition of association scheme will seem technical; in this section we offer one way of motivating it.

Let X be a graph with diameter d. The *distance graph* X_r has the same vertex set as X, but vertices u and v are adjacent in X_r if they are at distance exactly r in X. (Thus $X_1 = X$.) We use A_r to denote $A(X)r$ and find it convenient to use A_0 to denote I.

An automorphism of X can be viewed as a permutation matrix P that commutes with A_1. Clearly if P and A_1 commute, P must commute with each element of the adjacency algebra $\mathbb{R}[A_1]$ of X, that is, with any polynomial in A_1. However if P and A_1 commute, then P commutes with each matrix A_r and consequently P commutes with each element of the *distance algebra* $\mathcal{D}$ generated by $A_0, \ldots, A_d$. Since the distance algebra can be much larger than $\mathbb{R}[A_1]$, it can provide much stronger restrictions on the possible automorphisms of X. (If follows from the observations in 5.9 that, for almost graphs, $\mathcal{D}$ is the full matrix algebra.)

One problem here is that is not precisely clear what we meant when we wrote that $\mathcal{D}$ is 'larger' than $\mathbb{R}[A_1]$. We take the view that dimension is the right notion of size. In $|V(X)| = n$, then $\dim(\mathcal{D}) \leq n^2$ and, since the distance matrices $A_0, \ldots, A_d$ are linearly independent, we see that $\dim(\mathcal{D}) \geq d+1$. If $\mathcal{D}$ is $\mathrm{Mat}_{n\times n}(\mathbb{R})$, then the only permutation matrix that commutes with each of its elements if the identity, and therefore $\mathrm{Aut}(X)$ is trivial. Hence we might argue that X has the most 'regularity' when $\dim(\mathcal{D}) = d + 1$.

Let us consider the case $\dim(\mathcal{D}) = d + 1$ further. For any i, j such that $0 \leq i, j \leq d$, the product A_iA_j lies in $\mathcal{D}$; since $\mathcal{D}$ has a basis of symmetric matrices this implies that A_iA_j is symmetric, and therefore

$$A_jA_i = (A_iA_j)^T = A_iA_j.$$

Thus $\mathcal{D}$ is commutative. Since $J = \sum_r A_r$ lies in $\mathcal{D}$, each matrices A_i commutes with J and therefore the distance graphs $X_1, \ldots, X_d$ are regular.

The set of matrices

$$\{0, A_0, \cdots, A_d\}$$

is closed under Schur multiplication, from which we deduce that the algebra $\mathcal{D}$ that they generate is Schur-closed.

We restrict ourselves now to the case with $d = 2$ and $\dim(\mathcal{D}) = 3$. Here

$$A_2 = J - I - A_1$$

and therefore A_1 and A_2 commute if and only if A_1 and J commute, equivalently, if and only if X is regular. But much more is happening. For $\mathcal{D}$ contains all powers of A_1 and the matrices I, A_1 and A_1^2 are linearly independent (an easy exercise). Hence these three matrices are a basis for $\mathcal{D}$, which implies that any power of A_1 is a linear combination of I, A_1 and A_1^2 and therefore the minimal polynomial of A has degree three. We conclude that A_1 has exactly three eigenvalues (traditionally k, θ and τ) and its spectral decomposition is

$$A_1 = kE_0 + \theta E_1 + \tau E_2.$$

Since the spectral idempotents of A_1 are polynomials in A_1, they belong to $\mathcal{D}$. Since the spectral idempotents are linear independent, they form a second basis for $\mathcal{D}$. As $\mathcal{D}$ is Schur closed, the Schur products $E_i \circ E_j$ can be expressed as a linear combination of spectral idempotents.

To summarise, we have a matrix algebra $\mathcal{D}$ with a combinatorial basis A_0, A_1, A_2 of Shcur orthogonal ($A_i \circ A_j = 0$) Schur idempotents ($A_i \circ A_i = A_i$). It also has a basis E_0, E_1, E_2 of pairwise orthogonal matrix idempotents. In a sense, $\mathcal{D}$ is an algebra in two different ways.

14.2 Strongly Regular Graphs

We consider graphs with diameter two where $\dim(\mathcal{D}) = 3$ (which, in the next section, we will define to be *strongly regular graphs*). In this case, the matrices I, J and A are linearly independent, and therefore any power of A lies in their span. So there are constants k, a and c such that

$$A^2 = kI + aA + c(J - I - A).$$

We note that k is the valency of X. We write $\overline{A}$ for $J - I - A$. Then

$$A^2 - (a - c)A - (k - c)I = cJ$$

and as $(A - kI)J = 0$,

$$(A - kI)(A^2 - (a - c)A - (k - c)I) = 0.$$

It follows that

$$(t - k)(t^2 - (a - c)t - (k - c))$$

is the minimal polynomial of A, and its three zeros are the eigenvalues of A. (Since the diameter d is two, X has at least $d + 1 = 3$ distinct eigenvalues, so the minimal polynomial of A has degree three.)

Assume the eigenvalues of A are

$$k > \theta > \tau$$

Since X is connected and regular, k is a simple eigenvalue. If the multiplicities of θ and τ are respectively m_θ and m_τ and $n = |V(X)|$, then since

$$0 = \operatorname{tr}(A) = k + m_\theta \theta + m_\tau \tau$$

we deduce the equations

$$m_\theta + m_\tau = n - 1, \quad m_\theta \theta + m_\tau \tau = -k.$$

Solving these yields that

$$m_\theta = \frac{(n-1)\tau + k}{\tau - \theta}.$$

This surprisingly useful, providing a severe restriction on the possible parameter sets (k, a, c) for a strongly regular graph. (The expression for m_θ must reduce to a non-negative integer.) We also see that m_θ is determined by k, a and c.

We introduce a family of examples. A *Latin square* is an $n \times n$ matrix with entries from $\{1, \dots, n\}$ such that each integer occurs exactly once in each row and once in each column, e.g,

$$\begin{pmatrix} 0 & 1 & 2 & 3 \\ 1 & 2 & 3 & 0 \\ 2 & 3 & 0 & 1 \\ 3 & 0 & 1 & 2 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{pmatrix}$$

If L is an $n \times n$ Latin square, we can form. a graph with the n^2 triples

$$(i, j, L_{i,j}),\ 1 \le i, j \le n$$

as vertices, with two triples adajcent if they agree on one of the coordinates. If A is the adjacency matrix of an $n \times n$ Latin square,

$$A^2 = 3(n-1)I + (n+2)A + 6(J - I - A)$$

The eigenvalues are A are therefore $3n - 3$ and the zeros of

$$t^2 - (n-4)t - (3n-9) = (t+3)(t-n+1);$$

that is, $3n - 3$, $n - 1$, -3. Since the multiplicities of the eigenvalues are determined by the parameters, we infer that the two graphs coming from the $\times 4$ squares above are cospectral although, as it happens they are not isomorphic.

14.3 Axioms for Association Schemes

We introduce association schemes. We will see that if X has diameter d and its distance algebra has minimal dimension $d + 1$, then the distance matrices $A_0, \dots, A_d$ form an association scheme.

An *association scheme* $\mathcal{A}$ with d classes is a set of $n \times n$ 01-matrices $\{A_0, \dots, A_d\}$ such that:

(a) $A_0 = I$ and $\sum_r A_r = J$.

(b) $A_r^T \in \mathcal{A}$ for all r.

(c) For all r and s, the product $A_r A_s$ lies in the span of $\mathcal{A}$ over $\mathbb{C}$.

(d) $A_r A_s = A_s A_r$ for all r, s.

We can, and do, view the matrices $A_1, \ldots, A_d$ as the adjacency matrices of graphs $X_1, \ldots, X_d$ (with common vertex set), and we may view an association scheme as a set of d directed graphs. It follows from (a) and (d) that each matrix A_r commutes with J, and therefore these directed graphs are regular. An association scheme is *symmetric* if each matrix A_r is symmetric, when we have only graphs in sight. It is a traditional exercise to show that if each A_r is symmetric, then (d) is a consequence of the other axioms.

From (c) and (d), we see that the span of $\mathcal{A}$ is a commutative matrix algebra, known as the *Bose-Mesner algebra* of the scheme. Since the matrices A_r are 01-matrices that sum to J, they are linearly independent and so the dimension of the Bose-Mesner algebra is $d + 1$. This is the minimum possible dimension for a set of 01-matrices for which (a) holds.

Since the set consisting of $\mathcal{A}$ and the zero matrix is closed under Schur multiplication, the Bose-Mesner algebra of an association scheme is itself closed under Schur multiplication. This the Bose-Mesner algebra is an algebra with two multiplications; this is an extremely important property.

The matrices A_r are Schur idempotents, we refer to them as *primitive Schur idempotents*, since they cannot be expressed as nonzero sums of nonzero Schur idempotents from the Bose-Mesner algebra.

We consider examples. If $d = 1$, the only graph in the scheme is the complete graph K_n. If $d = 2$, the two graphs in the scheme are strongly regular; conversely a strongly regular graph and its complement give rise to an association scheme with two classes.

Another very relevant example is the Hamming scheme $H(n, q)$. We define this in terms of its graphs. Let Q be an alphabet with $|Q| = q$ and let $V = Q^n$. Let X_r be the graph with vertex set Q^n, where two n-tuples are adjacent in X if and only they are at Hamming distance r. We point out that in $H(n, 2)$ the graph X_1 is the n-cube and the graph X_1 in $H(n, q)$ is the *Hamming graph*—the n-th Cartesian power of K_n. Proving that the graphs X_r for an association scheme using just this definition and the axioms is a non-trivial task at this point. An easier but less direct approach is possible, as we now outline.

A permutation group G on a set V is *generously transitive* if, for each pair of points in V there is an element of G that swaps them. (For example, the dihedral group of order $2n$ acting on the cycle C_n.) You are invited to show that the non-diagonal orbitals of a generously transitive permutation group form a symmetric association scheme. Important note: in this case we can meet examples where the Schur idempotents A_r are **not** the distance matrices of some graph.

An association scheme is *primitive* if each of the graphs $X_1, \ldots, X_d$ is connected; otherwise it is *imprimitive*. Any union of the X_r's has equal in- and out-valency, hence it is weakly connected if and only if it is strongly connected.

We define a graph X to be *distance regular* if it is regular and the distance partition with any vertex is equitable. If X_r is a graph in an association scheme $\mathcal{A}$ with d classes, then the diameter of X_r is at most d. If equality holds we say that $\mathcal{A}$ is *metric* relative to X_r. If a scheme is metric, it is customary to have matters arranged so that the scheme is metric relative to X_1. It can be shown that $\mathcal{A}$ is metric relative to X_1 if and only if X_1 is distance regular. Strongly regular graphs are the distance-regular graphs of diameter two, more precisely they are the graphs that arise as the classes on association schemes with two classes.

14.4 Coherent Algebras

The Bose-Mesner algebra of an association scheme $\mathcal{A}$ is a commutative matrix algebra that contains J and is closed under transpose Schur-product. Any space of matrices closed under Schur product has a unique basis consisting of 01-matrices; these matrices are the adjacency matrices of the graphs that form $\mathcal{A}$. It is natural to consider what happens if we drop the assumption of commutativity.

A *coherent algebra* is a real or complex algebra of matrices that contains the all-ones matrix J and is closed under Schur multiplication, transpose and complex conjugation. A coherent algebra always has a basis of 01-matrices and this is unique, given that its elements are 01-matrices. This set of matrices determines a set of directed graphs and the combinatorial structure they form is referred to as a *coherent configuration*. When we say that a graph X is a "graph in a coherent algebra", we mean that $A(X)$ is a sum of distinct elements of the 01-basis.

A coherent algebra is *homogeneous* if the identity matrix is an element of its 01-basis. If M belongs to a homogeneous coherent algebra, then

$$M \circ I = \mu I$$

for some scalar μ. Hence the diagonal of any matrix in the algebra is constant. If A is a 01-matrix in the algebra, the diagonal entries of AA^T are the row sums of A. Therefore all row sums and all column sums of any matrix in the 01-basis are the same, and therefore this holds for each matrix in the algebra. In particular we can view the non-identity matrices as adjacency matrices of regular directed graphs. Any directed graph in a homogeneous coherent algebra must be regular. We note that if a coherent algebra is not homogeneous, then it is not commutative.

Any association scheme is a homogeneous coherent configuration. For a second class of examples we observe that if $\mathcal{P}$ is a set of permutation matrices of order $n \times n$, then the commutant of $\mathcal{P}$ in $\mathrm{Mat}_{n\times n}(\mathbb{C})$ is Schur-closed. Therefore it is a coherent algebra, and this algebra is homogeneous if and only the permutation group generated by $\mathcal{P}$ is transitive. Thus any graph whose automorphism group acts transitively on its vertices belongs to a coherent algebra.

Recall from Section 6.3 that a graph is walk regular if its vertex-deleted subgraphs $X \setminus u$ are all cospectral.

14.4.1 Lemma. *If X is a graph in a homogeneous coherent algebra, then X is walk regular.*

Proof. Any matrix in a coherent algebra is a linear combination of basis matrices, which are Schur orthogonal. If the algebra is coherent then one of the basis elements is I, and therefore any linear combination of basis elements has constant diagonal. inally, if A lies in a coherent algebra, so do all its powers. □

The graph in Figure 6.1 is walk regular but not vertex transitive. It does not lie in a homogeneous coherent algebra—the row sums of the Schur product

$$A \circ (A^2 - 4I) \circ (A^2 - 4I - J)$$

are not all the same.

A commutative coherent algebra is the same thing as a Bose-Mesner algebra of an association scheme. We will not go into this here, but we do note that the coherent algebra belonging to a distance-regular graph is commutative.

14.5 State Transfer on Coherent Algebras

The centre of a group is the set of elements in the group that commute with all elements of the group. The centre always contains the identity of the group, and if the group is the full symmetric group S_n with $n > 2$, then it consists exactly of the identity element only. On the other extreme, the centre of an abelian group is the entire group.

14.5.1 Theorem. *If X is a graph in a homogeneous coherent algebra with vertices u and v, and perfect state transfer from u to v occurs at time τ, then $U(\tau)$ is a scalar multiple of a permutation matrix with order two and no fixed points that lies in the centre of the automorphism group of X.*

Proof. First, if $A = A(X)$ where X is a graph in a homogeneous coherent algebra then, because it is a polynomial in A, the matrix $H(t)$ lies in the algebra for all t. Hence if

$$|H(\tau)_{u,v}| = 1$$

it follows that $H(\tau) = \xi P$ for some complex number ξ such that $|\xi| = 1$ and some permutation matrix P. Since A is symmetric, so is $H(t)$ for any t, and therefore P is symmetric. So

$$P^2 = PP^T = I$$

and P has order two. Since P has constant diagonal, its diagonal is zero and it has no fixed points. As P is a polynomial in A, it commutes with any automorphism of X and hence is central. □

This result should be compared with Theorem 1.11.1, which it generalizes considerably.

14.5.2 Corollary. *If X is a graph in a homogeneous coherent algebra with vertices u and v and there is perfect state transfer from u to v, then the number of vertices of X is even.*

Proof. Since $P^2 = I$ and the diagonal of P is zero, the number of columns of P is even. □

Saxena et al [52] `http://arxiv.org/abs/quant-ph/0703236` proved this corollary for circulant graphs.

A homogeneous coherent algebra is *imprimitive* if there is a non-identity matrix in its 01-basis whose graph is not connected, otherwise it is *primitive*. If the algebra is the commutant of a transitive permutation group, it is imprimitive if and only the group is imprimitive as a permutation group. The above corollary implies that if perfect state transfer takes place on a graph from a homogeneous coherent algebra, the algebra is imprimitive.

Note that this corollary holds for any vertex-transitive graph, and for any distance-regular graph.

14.6 Spectral Decomposition of Schemes

Any matrix in an association scheme is normal, and so it has a spectral decomposition. It is more convenient to define a decomposition for the entire Bose-Mesner algebra.

Since the Bose-Mesner algebra is commutative and each matrix in it is normal, we may consider the set $\mathcal{E}$ of all possible products of the spectral idempotents of the matrices A_r. Each nonzero element of $\mathcal{E}$ is an idempotent and belongs to the Bose-Mesner algebra of the scheme. If E and F are idempotents, we write $E \le F$ if $EF = E$. With respect to this ordering the minimal non-zero idempotents are orthogonal. It can be shown that they form a basis for the Bose-Mesner algebra, whence there are exactly $d+1$ minimal nonzero idempotents in $\mathcal{E}$. We denote them by $E_0, \ldots, E_d$ and note that they satisfy the following:

(a) $\frac{1}{n}J \in \{E_0, \ldots, E_d\}$, $\sum E_r = I$.

(b) $\overline{E_r} = E_s$ for some s.

(c) $E_r \circ E_s$ lies in the span of $E_0, \ldots, E_d$.

It is conventional to assume that $E_0 = \frac{1}{n}J$. We note that (b) holds because the Bose-Mesner algebra has a real basis and that (c) holds because the Bose-Mesner algebra is closed under Schur multiplication. We will refer to the matrices E_r as the *primitive spectral idempotents*.

If $M \in \mathbb{C}[\mathcal{A}]$, there is a constant λ_M such that $ME_r = \lambda_M E_r$; thus the columns of E_r are eigenvectors for M, all with the same eigenvalue. Therefore there are scalars $p_r(s)$ such that $A_r E_s = p_r(s) E_s$ and

$$A = \sum_s p_r(s) E_s.$$

The scalars $p_r(s)$ for $s = 0, \dots, d$ are eigenvalues of A, and we refer to the matrix P defined by

$$P_{r,s} := p_s(r)$$

as the *matrix of eigenvalues* of the scheme.

For fixed r, the matrices $E_r \circ A_s$ are linearly independent, and it follows that $E_r \circ A_s$ must be a scalar multiple of A_s. If our scheme has n vertices, there must be scalars $q_r(s)$ such that

$$E_s = \frac{1}{n} \sum_r q_s(r) A_r.$$

The matrix Q given by

$$Q_{r,s} := q_s(r)$$

is the *matrix of dual eigenvalues* of the scheme. We have

$$PQ = nI.$$

There is a second relation betwen P and Q. Let Δ_m be the diagonal matrix of order $(d+1) \times (d+1)$ with i-th diagonal entry equal to $\operatorname{rk}(E_i)$ and let Δ_v denote the diagonal matrix of order $(d+1) \times (d+1)$ with i-th diagonal entry equal to v_r, the row sum of A_r. Then

$$P \Delta_m P^* = n \Delta_v \tag{14.6.1}$$

and thus the matrix

$$\Delta_v^{-1/2} P \Delta_m^{1/2}$$

is orthogonal.

Since the product $A_r A_s$ lies in the span of $\mathcal{A}$, there are scalars $p_{r,s}(j)$ such that

$$A_r A_s = \sum_j p_{r,s}(j) A_j.$$

Since all matrices A_r are 01-matrix it is immediate that the number $p_{r,s}(j)$ are non-negative integers. In fact $p_{r,s}(j)$, for any pair (a, b) of j-related vertices, $p_{r,s}(j)$ counts the number of vertices that are r-related to a and s-related to b. If v_s denotes the sum of a row of A_s, then the quantity

$$v_s p_{r,s}(j)$$

is invariant under permutations of r, s and j—because this number counts the triangles of vertices with sides of "length" r, s and j that contain a gieven vertex.

Naturally there are parameters "dual" to the intersection number, known as the *Krein parameters* of the scheme. These are the numbers $q_{r,s}(j)$ such that

$$E_r \circ E_s = \frac{1}{n} \sum_j q_{r,s}(j) E_j.$$

These numbers are not always integers, and hence have no natural combinatorial interpretation. However $q_{r,s}(j)/n$ is an eigenvalue of $E_r \circ E_s$, and therefore it is real. Since the Schur product of positive semidefinite matrices is positive semidefinite, the Krein parameters are also non-negative.

14.7 Translation Schemes

Suppose G is a finite group with conjugacy classes $C_0, \ldots, C_d$, where $C_0 = \{1\}$. Define X_r to be the directed graph with vertex set G, with elements g and h adjacent in X_r if $hg^{-1} \in C_r$. (In other terms, X_r is the Cayley graph $X(G, C_r)$. (Here we allow a Cayley graph to be a directed graph, the connection set need not be inverse-closed.) Then the directed graphs $X_1, \ldots, X_d$ form an association scheme, the *conjugacy class scheme* of the group G. We leave the details as an exercise. When G is abelian, each conjugacy class has size one, and the matrices A_r are permutation matrices. In this case we call the conjugacy class scheme a *translation scheme*.

Any graph constructed as the union of a subset of the classes $X_1, \ldots, X_d$ from a conjugacy class scheme is a Cayley graph for the underlying group. Such Cayley graphs are known as *normal Cayley graphs* and are characterized by the property that their connection sets are unions of onjugacy classes. When G is abelian, we refer to the Cayley graphs as *translation graphs*.

One nice feature of conjugacy class schemes is that we can give something like an explicit form for their primitive spectral idempotents:

14.7.1 Lemma. *Suppose ψ is an irreducible representation of the group G and M_ψ is the matrix with rows and columns indexed by G such that*

$$(M_\psi)_{g,h} = \psi(hg^{-1})$$

Then the matrices

$$E_\psi = \frac{\psi(1)}{|G|} M_\psi$$

are the primitive spectral idempotents of the conjugacy class scheme of G. □

For translation schemes we can be more explicit, because we can give the eigenvectors explicitly. If ψ is a character of the G, then ψ is an eigenvector for the Bose-Mesner algebra of the scheme. We have

$$E_\psi = \psi\psi^*,$$

this is a consequence of the previous lemma, but is very easy to verify directly.

In a translation scheme we may denote the primitive Schur idempotents by A_g, for g in G, with

$$A_g A_h = A_{gh}.$$

(Each A_g is a permutation matrix.) If ψ is a character and $S \subseteq G$, then define

$$\psi(S) := \sum_{g \in S} \psi(g).$$

14.7.2 Lemma. *Suppose $X = X(G, C)$ is a translation graph for the abelian group G and $A = A(X)$. If ψ is a character for G, then*

$$A\psi = \psi(C)\psi.$$ □

If $\mathcal{A}$ is the scheme of the cyclic group of order v and θ is a primitive v-th root of 1 then we may assume that

$$P_{i,j} = \theta^{(i-1)(j-1)}. \tag{14.7.1}$$

Note that this matrix is symmetric, It is easy to verify that $P\overline{P} = nI$, whence $Q = \overline{P}$. If G is abelian then G can be expressed as the direct product of cyclic groups, and its matrix of eigenvalues can be written as a Kronecker products of matrices of the same form as P. Hence if P is the matrix of eigenvalues of a translation scheme, we may assume that P is symmetric and $\overline{P} = Q$.

14.8 Integral Subschemes

Suppose $\mathcal{A} = \{A_0, \ldots, A_d\}$ and $\mathcal{B} = \{B_0, \ldots, B_e\}$ are association schemes on the same vertex set. We say that $\mathcal{B}$ is a *subscheme* of $\mathcal{A}$ if each matrix B_r is a sum of matrices from $\mathcal{A}$ (necessarily $B_0 = A_0 = I$). Subschemes are also known as *fusion schemes*. Trivial examples is provided by the association scheme of the complete graph K_n, which is a subscheme of any scheme on n vertices.

We consider a more interesting class of examples. Consider the subspace of the Bose-Mesner algebra $\mathbb{C}[\mathcal{A}]$ spanned by the matrices with only rational entries and rational eigenvalues. This algebra contains I and J and is closed under both matrix and Schur multiplication. It follows that it is the Bose-Mesner algebra of an association scheme $\mathcal{B}$, and this scheme is a subscheme of $\mathcal{A}$. Since the eigenvalues of an integer matrix are algebraic integers, it follows that the integer matrices in $\mathbb{C}[\mathcal{B}]$ have only integer eigenvalues. We call $\mathcal{B}$ the *integral subscheme* of $\mathcal{A}$.

We can provide a concrete description of the integral subscheme of the scheme of an abelian group. Suppose G is abelian and, if $g \in G$, let A_g be the permutation matrix that represents multiplication by g on $\mathbb{C}[G]$. Thus the matrices A_g are the minimal Schur idempotents of the group scheme. The characters of G form a group G^* isomorphic to G, and we use ψ_g to denote the image in G^* of the element g of G. Define a relation $\approx$ on G by by declaring that $g \approx h$ if and only $\langle g \rangle = \langle h \rangle$, i.e., g and h generate the same cyclic subgroup of G. We observe that $\approx$ is an equivalence relation on the elements of G, and the number of equivalence classes is the number of cyclic subgroups of G. We have the following important result due to Bridges and Mena.

14.8.1 Theorem. *If $X = X(G, C)$ is a Cayley graph for the abelian group G, then its eigenvalues are all integers if and only if C is $\approx$-closed.*

Proof. Let $[x]$ denote the $\approx$-class of x. (This consists of all generators of the cyclic group $\langle x \rangle$.) We claim that if ψ is a character of G, then $\psi([x]) \in \mathbb{Z}$; this implies that the stated condition is sufficient.

The key is that if $H \leq G$ and $\psi \in G^*$ then either $H \leq \ker(\psi)$ (and $\psi(h) = 1$ for all h in H) or $\psi(H) = 0$. To prove this, choose h in H and note that

$$\psi(H) = \psi(hH) = \psi(h)\psi(H),$$

whence either $\psi(h) = 1$ or $\psi(H) = 0$.

Suppose x in G has order m and $\psi \in G^*$. If $x \in \ker(\psi)$ then $\psi([x]) = m$. If $x \in ker(\psi)$, then $[x] \subseteq \ker(\psi)$, and if $x \notin \ker(\psi)$ then

$$[x] \cap \ker(\psi) = \emptyset.$$

Since $\langle x \rangle$ is cyclic and $[x]$ is the set of generators of $\langle x \rangle$, it follows that $\langle x \rangle \setminus [x]$ is a subgroup of $\langle x \rangle$. Therefore

$$\psi(\langle x \rangle \setminus [x]) \in \mathbb{Z}$$

and it follows that $\psi([x])$ must be an integer.

Assume now that $\psi(C)$ is an integer for all characters ψ; we must deduce that C is $\approx$-closed. Assume that the exponent of G is m. Then

$$1 = \psi(0) = \psi(mx) = \psi(x)^m$$

and so all character values are m-th roots of 1. Let Γ be the group of units of $\mathbb{Z}_m$. Note that if $\mathbb{F}$ is the extension of $\mathbb{Q}$ generated by a primitive m-th root of 1, then Γ is the Galois group of this extension. If $a \in \Gamma$ then the map $x \mapsto ax$ is an automorphism of G. If for a character ψ we define ψ^a by

$$\psi^a(x) := \psi(ax)$$

then Γ also acts as a group of automorphisms of G^*. (This means we have three distinct actions of Γ: on G, on G^* and as a Galois group.)

Since the eigenvalues of X are integers

$$\psi^a(C) = \psi(C)$$

for all a in Γ and therefore

$$\psi(aC) = \psi(C)$$

for all a. As this holds for all characters, it follows that $aC = C$ and consequently C is $\approx$-closed. □

One consequence of this result is that a Cayley graph for an abelian group whose exponent divides 4 or 6 will have integer eigenvalues.

Our relation $\approx$ is also an equivalence relation on G^*. If $g \mapsto \psi_g$ is an isomorphism from G to G^*, then $g \approx h$ if and only if $\psi_g \approx \psi_h$. Therefore there is a bijection between the $\approx$-classes of G and those of G^*, and this bijection preserves the size of a class. Hence, using the notation from Section 14.6, we may assume that $\Delta_m = \Delta_v$.

14.9 Perfect State Transfer on Distance-Regular Graphs

The paper Coutinho et al [22] provides a close to complete list of the distance-regular graphs that admit perfect state transfer. We discuss some the results from this paper. The standard reference is Brouwer, Cohen and Neumaier [14]; there is also an introduction in [35].

A distance-regular graph is *antipodal* if its diameter is d and the relation on vertices "is equal to or at distance d from" is an equivalence relation. The equivalence classes are called *fibres*. If a distance-regular graph is antipodal, the fibres all have same size. The d-cubes are antipodal distance-regular graphs with fibres of size two; the line graph of the Petersen graph is antipodal with fibres of size three. The cocktail party graph $\overline{mK_2}$ is strongly regular with diameter two.

The partition of a distance-regular graph into antipodal fibres is necessarily equitable, and the resulting quotient graph is distance regular but not antipodal. The distance-regular graph is a cover of its quotient—the vertices in distinct fibles are either not adjacent or are paired by a matching. If the graph has diameter d, the quotient has diameter $\lfloor d/2 \rfloor$.

If a distance-regular graph admits pst, then it must be antipodal. Although this condition rules out many graphs, it still leaves considerable scope.

A distance-regular graph of diameter one is a complete graph, and K_2 is the only complete graph that admits pst.

14.9.1 Lemma. *If perfect state transfer occurs on the distance-regular graph X, then either X is K_2 or $\overline{mK_2}$, or the diameter of X is at least three and X is antipodal with all fibres of size two.*

Proof. Let π be the distance partition of X relative to a vertex a, with cells $C_0, \ldots, C_d$. Then the sequence of cell sizes $|C_r|$ (for $r = 0, \ldots, m$) is unimodal. By Lemma **??**, if we have pst from a to b, then $\{b\}$ must be a cell of π, and therefore X is antipodal with fibres of size two, and b is the unique vertex in X at distance d from a. We leave it as an exercise to show that an antipodal strongly regular graph must be isomorphic to $\overline{mK_2}$. □

Note that both K_2 and the cocktail party graphs admit perfect state transfer.

An antipodal distance-regular graph of diameter three is a cover of a complete graph, and the graphs of diameter three with antipodal classes of size two are necessarily switching graphs, as discussed in Section 12.7. The eigenvalues of a distance-regular 2-fold cover of K_n are

$$n-1,\ -1,\ \theta,\ \tau$$

where $\theta\tau = 1-n$. We say that θ and τ are the non-trivial eigenvalues of the cover. There are many classes of such covers that admit pst, and these are discussed in [22]. Here we consider just one interesting family.

14.9.2 Lemma. *If X is a distance-regular 2-fold cover of K_n with non-trivial eigenvalues θ and τ. If $\theta+\tau=-2$, then X admits perfect state transfer at time $\pi/\sqrt{n}$.* □

One feature of this class of examples is that the time to pst is so short. The infinite families of distance-regular graphs that admit pst are:

(a) The d-cubes.

(b) The halved d-cubes.

(c) The Hadamard graphs or order n, where n is a perfect square.

The d-cubes we have met. The *halved d-cube* is the graph with a colour class of Q_d as its vertices, and with two such vertices adjacent if and only if they are at distance two in the d-cube. (So it has 2^{d-1} vertices and valency $\binom{d}{2}$). We will meet these graphs again when we study uniform mixing in Chapter 17.) A *Hadamard graph* is construct from an $n\times n$ Hadamard matrix as follows. Write H as

$$H = H_0 - H_1$$

where H_0 and H_1 are 01-matrices, and then define

$$B = H_0 \otimes \begin{pmatrix}1&0\\0&1\end{pmatrix} + H_1 \otimes \begin{pmatrix}0&1\\1&0\end{pmatrix}.$$

The Hadamard graph associated with H is the bipartite graph with adjacency matrix

$$\begin{pmatrix}0&B\\B^T&0\end{pmatrix}.$$

It is bipartite with diameter four, and antipodal with fibres of size two. (It is a double cover of the complete bipartite graph $K_{n,n}$.)

Finally we note that in [22] there are many examples of distance-regular graphs X such that the direct product $K_2 \times X$ admits perfect state transfer. Here X may even be strongly regular.

14.10 Duality

We will make use of the results in this section in Chapter 17, when we study mixing on translation graphs.

Let $\mathcal{A}$ be an association scheme. A subspace of its Bose-Mesner algebra is the Bose-Mesner algebra of an association scheme if it closed under matrix and Schur multiplication and contains I and J. (The key observation is that a Schur-closed subspace must have a basis of 01-matrices.) An association scheme obtained in this way is said to be a *subscheme* (or *fusion scheme*.) Each primitive idempotent of a subscheme of $\mathcal{A}$ is sum of primitive Schur idempotents of $\mathcal{A}$. For example, the Hamming scheme $H(d,2)$ is a subscheme of the translation scheme belonging to $\mathbb{Z}_2^d$.

We say an association scheme $\mathcal{A}$ is *formally self-dual* if $Q = \overline{P}$.

If $r \in \{0, 1, \ldots, d\}$, we define r^T to be the element of $r \in \{0, 1, \ldots, d\}$ such that $A_{r^T} = A_r^T$. We recall that $p_r(k) = \overline{p_r(k^T)}$.

14.10.1 Theorem. *Let $\mathcal{A}$ be a formally self-dual association scheme on n vertices and let Θ be the linear mapping from $\mathbb{C}[\mathcal{A}]$ to itself such that $\Theta(A_r) = \sum_r p_r(j) A_r$. Then:*

(a) $\Theta(A_r) = n\overline{E_r}$.

(b) $\Theta(I) = J$, $\Theta(J) = nI$.

(c) $\Theta^2(M) = nM^T$ *for all* M *in* $\mathbb{C}[\mathcal{A}]$.

(d) $\Theta(MN) = \Theta(M) \circ \Theta(N)$ *for all* M *and* N *in* $\mathbb{C}[\mathcal{A}]$.

(e) $\Theta(M \circ N) = \frac{1}{n}\Theta(M)\Theta(N)$ *for all* M *and* N *in* $\mathbb{C}[\mathcal{A}]$.

(f) If $\mathcal{B}$ is a subscheme of $\mathcal{A}$, then $\Theta(\mathcal{B})$ is also a subscheme of $\mathcal{A}$.

Proof. Since $\overline{p_r(j)} = q_r(j)$, we have

$$\Theta(A_r) = \sum_{j=0}^{d} \overline{q_r(j)} A_r = n\overline{E_r}.$$

In particular, $\Theta(I) = J$.

Next

$$\Theta(n\overline{E_r})) = \sum_r \overline{q_r(j)}\Theta(A_r) = \sum_{j,k} \overline{q_r(j)} p_r(k) A_k = \sum_{j,k} q_r(j) p_r(k^T) A_k^T.$$

Since $QP = nI$, it follows that $\Theta(nE_r) = nA_r^T$ and hence

$$\Theta^2(M) = nM^T \tag{14.10.1}$$

for all M in $\mathbb{C}[\mathcal{A}]$. (Note that $\Theta(J) = nI$.)

Since the entries of $\Theta(A_r)$ are the eigenvalues of A_r, we see that $\Theta(A_r A_r) = \Theta(A_r) \circ \Theta(A_r)$ and hence

$$\Theta(MN) = \Theta(M) \circ \Theta(N), \tag{14.10.2}$$

for all M and N in $\mathbb{C}[\mathcal{A}]$.

Finally

$$\Theta(A_r \circ A_r) = \delta_{i,j} n\overline{E_r} = \frac{1}{v}\Theta(A_r)\Theta(A_r).$$

and thus

$$\Theta(M \circ N) = \frac{1}{n}\Theta(M)\Theta(N). \tag{14.10.3}$$

for all M and N in $\mathbb{C}[\mathcal{A}]$. □

If Θ is a map satisfying the conditions of this theorem, we call it a *duality map* on $\mathcal{A}$. The matrix representing Θ relative to the basis $A_0, \dots, A_d$ is P. From (c) in the theorem we see that Θ commutes with transpose, that is

$$\Theta(M^T) = \Theta(M)^T.$$

It seems reasonable to define an association scheme on v vertices to be *self-dual* if there is an endomorphism Θ of $\mathrm{Mat}_{n\times n}(\mathbb{C})$ such that $\Theta(A_r) = v\overline{E_r}$ for $i = 0, 1, \dots, d$.

If $\mathcal{A}$ and $\mathcal{B}$ are schemes and the matrix of eigenvalues of $\mathcal{B}$ is the complex conjugate of the matrix of dual eigenvalues of $\mathcal{A}$, we say that $\mathcal{A}$ and $\mathcal{B}$ are *formally dual*. In this case we can define a map Θ as above, and a slightly modified version of 14.10.1 still holds. If Θ is induced by an endomorphism of $\mathrm{Mat}_{n\times n}(\mathbb{C})$, we say the pair of schemes is *dual*.

14.11 Type-II Matrices

If M is a matrix over a field with no entry zero, we denote its *Schur inverse* by $M^{(-T)}$, thus $M \circ M^{(-T)} = J$. A complex $n \times n$ matrix is a *type-II matrix* if it is Schur invertible and

$$MM^{(-T)} = nI.$$

Hadamard matrices provide us with many examples. For another family of simple examples, consider the $n \times n$ matrix

$$M = (t-1)I + J$$

for which $M^{(-T)} = (t^{-1} - 1)I + J$. Then

$$MM^{(-T)} = (2 - t - t^{-1})I + (n - 2 + t + t^{-1})J$$

and therefore M is a type-II matrix if $t^2 + (n-2)t + 1 = 0$, that is, if

$$t = \frac{1}{2}(2 - n \pm \sqrt{n^2 - 4n}).$$

These matrices are known as *Potts models*.

The Kronecker product of two type-II matrices is a type-II matrix.

The unitary type-II matrices form an important special class, whose members are often referred to as *complex Hadamard matrices*.

14.11.1 Theorem. *Let M be a square complex matrix. Then any two of the following statements imply the third:*

(a) M is a type-II matrix.

(b) M is flat.

(c) Some scalar multiple of M is unitary.

We define a *monomial matrix* be to a product of an invertible diagonal matrix with a permutation matrix. The set of all $n \times n$ matrices forms a group, the *monomial group*. We say that matrices M and N are *monomially equivalent* if there are monomial matrices R and S such that $N = RMS$. It is easy to verify that if matrices M and N are monomially equivalent and M is type-II, then N is type-II. If M is type-II then so is M^T but, in general, they need not be equivalent.

14.12 Type-II Matrices in Schemes

The type-II matrices that interest us here will be flat, and will belong to the Bose-Mesner algebra of an association scheme. The Bose-Mesner algebra of a scheme will always contain a Potts model, so the question is what other type-II matrices might be present.

14.12.1 Lemma. *Suppose $\mathcal{A}$ is an association scheme. Then the type-II matrices in the Bose-Mesner algebra of $\mathcal{A}$ form an algebraic variety defined by polynomials with integer coefficients.*

Proof. Suppose the basic Schur idempotents in $\mathcal{A}$ are $A_0, \dots, A_d$ and set

$$W = \sum_r x_r A_r.$$

Assume that $A_r^T = A_{r'}$. Then

$$WW^{(-)T} = \sum_{r,s} x_r x_s^{-1} A_r A_{s'}$$

and therefore W is type-II if and only if, for $k = 1, \dots, d$,

$$\sum_{r,s'} x_r x_{s'}^{-1} p_{r,s'}(k) = 0.$$

Since the intersection number $p_{r,s'}(k)$ are integers, it follows that the set of solutions of this system of polynomial equations forms an algebraic variety and the coefficients of these polynomials are integers. □

14.12.2 Corollary. *If the number of type-II matrices with diagonal entries 1 in the Bose-Mesner algebra of an association scheme is finite, then the entries of these matrices are algebraic integers.* □

14.12.3 Theorem. *If Θ is a duality map on the formally self-dual association scheme $\mathcal{A}$ and M is a type-II matrix in the Bose-Mesner algebra of the scheme, then $\Theta(M)$ is type-II. If M is flat then $\Theta(M)$ is a scalar multiple of a unitary matrix. If M is unitary, $\Theta(M)$ is flat.*

Proof. Suppose M is type-II. Then $MM^{(-T)} = nI$, whence $M^{(-T)} = nM^{-1}$ and so

$$J = M \circ M^{(-)} = nM \circ (M^{-1})^T.$$

Therefore

$$nI = \Theta(J) = \Theta(nM \circ (M^{-1})^T) = n\Theta(M)\Theta((M^{-1})^T),$$

and from Theorem 14.10.1(d) we have that $\Theta(M^{-1}) = \Theta(M)^{(-)}$, and we conclude that $\Theta(M)$ is a type-II matrix.

Suppose $M \in \mathbb{C}[\mathcal{A}]$ and

$$M = \sum_r \mu_r E_r.$$

Then

$$M^* = \sum_r \overline{\mu_r} E_r^* = \sum_r \overline{\mu_r} E_r$$

and we see that M is unitary if and only if its eigenvalues have norm 1. The second claim follows. □

14.13 Type-II Matrices from Strongly Regular Graphs

We work out the conditions for a matrix $I + xA + y\overline{A}$ in the Bose-Mesner algebra of a strongly regular graph. This serves as a concrete example for the theory in the previous section, and we will also use the result when we study uniform mixing on conference graphs in Section 17.5.

14.13.1 Lemma. *Let X be a strongly regular graph with parameters $(n, k; a, c)$. If*

$$W = I + xA + y\overline{A}$$

then W is a type-II matrix if and only if x and y satisfy

$$n - 2k + 2a + (k - a - 1)(xy^{-1} + x^{-1}y) + x + x^{-1} = 0 \qquad (14.13.1)$$

$$n - 2k + 2c - 2 + (k - c)(xy^{-1} + x^{-1}y) + y + y^{-1} = 0. \qquad (14.13.2)$$

Proof. We have

$$A^2 = kI + aA + c\overline{A}$$

and since $\overline{X}$ is strongly regular with parameters

$$n,\ n - 1 - k,\ n - 2 - 2k + c,\ n - 2k + a$$

we also have

$$\overline{A}^2 = (n-1-k)I + (n-2-2k+c)\overline{A} + (n-2k+a)A.$$

Further

$$A\overline{A} = (k-1-a)A + (k-c)\overline{A}.$$

If $W = I + xA + y\overline{A}$ for non-zero complex numbers x and y, then

$$\begin{aligned} WW^{(-T)} &= (I + xA + y\overline{A})(I + x^{-1}A + y^{-1}\overline{A}) \\ &= I + A^2 + \overline{A}^2 + (x + x^{-1})A + (y + y^{-1})\overline{A} + (xy^{-1} + x^{-1}y)A\overline{A}. \end{aligned}$$

We see that the coefficient of A in this expression is equal to the left side of (14.13.1) and the coefficient of $\overline{A}$ is equal to the left side of (14.13.2). □

Notes

Exercises

Chapter 15

Average Mixing

As we noted when we defined the transition matrix $U_X(t)$, although it determines a physical process what we can actually observe are the entries of

$$M_X(t) := U_X(t) \circ \overline{U_X(t)} = U_X(t) \circ U_X(-t).$$

We call M_X the *mixing matrix* belonging to X. Since $U_X(t)$ is unitary then entries of $M_X(t)$ are non-negative reals that sum to 1 along each row and along each column. Thus each row and each column is a probability density. Since $M_X(t)$ is a principal submatrix of a unitary matrix, it is necessarily a contraction.

15.1 Average Mixing

We define the *average mixing matrix* of X by

$$\widehat{M}_X := \frac{1}{T}\int_0^T M_X(t)\,dt.$$

Since the mixing matrix $M_X(t)$ is doubly stochastic for all t, the average mixing matrix is also doubly stochastic.

15.1.1 Theorem. *Let A be the adjacency matrix of X. If A has spectral decomposition $A = \sum \theta_r E_r$ then*

$$\widehat{M}_X = \sum_r E_r^{\circ 2}.$$

Proof. We have

$$\begin{aligned} M_X(t) &= \sum_{r,s} e^{i(\theta_r-\theta_s)t} E_r \circ E_s \\ &= \sum_r E_r^{\circ 2} + 2\sum_{r>s} \cos((\theta_r-\theta_s)t)\, E_r \circ E_s. \end{aligned}$$

The theorem now follows from the observation that

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \cos(\varphi t)\,dt = 0. \qquad \square$$

We note two properties of the mixing matrix that will prove useful.

15.1.2 Lemma. *We have* $I \succcurlyeq M_X(t) \succcurlyeq 2\widehat{M}_X - I$.

Proof. From the above

$$M_X(t) = \sum_r E_r^{\circ 2} + 2\sum_{r>s} \cos((\theta_r-\theta_s)t)\, E_r \circ E_s$$

and, since $I = \sum_r E_r$ and $I \circ I = I$, we also have

$$I = \sum_r E_r^{\circ 2} + 2\sum_{r>s} E_r \circ E_s.$$

Therefore

$$I - M_X(t) = 2\sum_{r>s}(1-\cos((\theta_r-\theta_s)t))\, E_r \circ E_s$$

where, by a theorem of Schur, the matrices $E_r \circ E_s$ are positive semidefinite. If follows that $I - M_X(t) \succcurlyeq 0$. Similarly

$$M_X(t) + I = 2\widehat{M}_X + 2\sum_{r>s}(1+\cos((\theta_r-\theta_s)t))\, E_r \circ E_s$$

where the sum is positive semidefinite, and so $M_X(t) \succcurlyeq 2\widehat{M}_X - I$. $\square$

One consequence of this lemma is that all eigenvalues of $M_X(t)$ lie in the interval $[-1,1]$ (don't forget that $M(t)$ is symmetric). As an exercise you may prove that if pst occurs at time t, then -1 is an eigenvalue of $M_X(t)$. A second proof that the eigenvalues of $M(t)$ lie in $[-1,1]$ comes from the following.

15.1.3 Lemma. *If M is a principal submatrix of a unitary matrix, then* $\|Mz\| \le \|z\|$ *for any vector* z. $\square$

Equivalently, we may say that a principal submatrix of a unitary matrix is a *contraction*. Clearly all eigenvalues of a contraction lie in $[-1,1]$.

15.2 Properties of the Average Mixing Matrix

In this section we derive some basis properties of the average mixing matrix. We know already that it is symmetric. By a famous theorem of Schur, the Schur product $M \circ N$ of two positive semidefinite matrices is positive semidefinite and, since the sum of positive semidefinite matrices is positive semidefinite, we see that $\widehat{M}_X$ is positive semidefinite. If A and B are symmetric matrices of the same order, we write $A \succcurlyeq B$ to denote that $A - B$ is positive semidefinite.

Clearly $\widehat{M}_X$ is a nonnegative matrix. In fact:

15.2.1 Lemma. *If X is connected, all entries of $\widehat{M}_X$ are positive.*

Proof. Each Schur square $E_r^{\circ 2}$ is nonnegative and if $(\widehat{M}_X)_{u,v} = 0$ then $(E_r^{\circ 2})_{u,v} = 0$. However this implies that $(E_r)_{u,v} = 0$ for all r and hence any linear combination of the idempotents E_r has uv-entry zero. Since this implies that $(A^k)_{u,v} = 0$ for all k we conclude that X is not connected. □

In the next secion we show that average mixing is never uniform, that is, $\widehat{M}_X$ cannot be a scalar multiple of the all-ones matrix J.

15.2.2 Lemma. *If $\widehat{M}_X$ is the average mixing matrix of the graph X then all eigenvalues of $\widehat{M}_X$ lie in the interval* $[0, 1]$.

Proof. Since $\widehat{M}_X \succcurlyeq 0$, its eigenvalues are non-negative. For the upper bound, we note that

$$I = I \circ I = \left(\sum_r E_r \right)^{\circ 2} = \widehat{M}_X + 2 \sum_{r<s} E_r \circ E_s.$$

Since the final sum here is positive semidefinite, it follows that $I - \widehat{M}_X \succcurlyeq 0$. Therefore all eigenvalues of $\widehat{M}_X$ are in $[0, 1]$. □

Since $\widehat{M}_X$ is the average of doubly stochastic matrices, it is doubly stochastic and its largest eigenvalue is 1. We can also see this without appealing to the averaging. Notice that

$$\begin{aligned}((E_r \circ E_r)\mathbf{1})_u &= ((e_u^T E_r) \circ (e_u^T E_r))\mathbf{1} \\ &= \langle e_u^T E_r, e_u^T E_r \rangle \\ &= e_u^T E_r^2 e_u \\ &= e_u^T E_r e_u \\ &= (E_r)_{u,u}\end{aligned}$$

and, since $\sum_r E_r = I$, it follows that $\widehat{M}_X \mathbf{1} = \mathbf{1}$.

15.2.3 Lemma. *The entries of the average mixing matrix of a graph are rational.*

Proof. Let $\phi(X, x)$ be the characteristic polynomial of X, and let $\mathbb{F}$ be a splitting field for $\phi(X, x)$. We use the fact that an element of $\mathbb{F}$ which is fixed by all field automorphisms of $\mathbb{F}$ must be rational. If σ is an automorphism of $\mathbb{F}$, then

$$A = A^\sigma = \sum_r \theta_r^\sigma E_r^\sigma.$$

Since θ_r^σ must be an eigenvalue of A and since the spectral decomposition of A is unique, it follows that E_r^σ is one of the idempotents in the spectral decomposition of A. Therefore the set of idempotents is closed under field automorphisms, and so must the $\{E_r^{\circ 2}\}_r$. Consequently

$$\widehat{M}_X^\sigma = \widehat{M}_X$$

for all σ and therefore $\widehat{M}_X$ is rational. □

Note that this lemma holds whether we use the Laplacian or the adjacency matrix—all we need is that A be symmetric with integer entries.

We use $L(X)$ to denote the Laplacian matrix X. If Δ is the diagonal matrix whose i-th diagonal entry is the valency of the i-vertex of X, then

$$L(X) = \Delta - A.$$

The transition matrix of X relative to $L(X)$ is

$$U_L(t) := \exp(it(\Delta - A)).$$

When X is regular, questions about U_L reduce immediately to questions about U_X, but in general there is no simple relation between the two cases.

15.2.4 Lemma. *If X is regular and X and its complement $\overline{X}$ are connected, then X and $\overline{X}$ have the same average mixing matrix. For any graph X, the average mixing matrix relative to the Laplacian of X is equal to the average mixing matrix relative to the Laplacian of $\overline{X}$.*

Proof. If X is regular then the idempotents in the spectral decomposition of its adjacency matrix are the idempotents in the spectral decomposition of the adjacency matrix of $\overline{X}$. For any graph X on n vertices

$$L(\overline{X}) = L(K_n) - L(X);$$

since $L(K_n) = nI - J$ and since $L(X)$ commutes with J, the idempotents in the spectral decomposition of its Laplacian are the idempotents in the spectral decomposition of the Laplacian of $\overline{X}$. □

15.3 Uniform Average Mixing?

15.3.1 Lemma. *If $\widehat{M}_X$ is the average mixing matrix of the graph X on n vertices and m_r is the dimension of the r-th eigenspace of X, then*

$$\operatorname{tr}(\widehat{M}_X) \geq \frac{1}{n}\sum_r m_r^2.$$

Equality holds if and only if X is walk regular.

Proof. Let $E_1, \ldots, E_m$ be the spectral idempotents of X. The diagonal entries of E_r are non-negative and their sum is m_r, the dimension of the r-th eigenspace. Hence

$$\operatorname{tr}(E_r^{\circ 2}) \geq \frac{m_r^2}{n}.$$

and therefore

$$\operatorname{tr}(\widehat{M}_X) \geq \sum_r \frac{m_r^2}{n}.$$

If equality, holds then the diagonal entries of E_r are equal to m_r/n. Hence each idempotent has constant diagonal. Therefore all powers of A have constant diagonal, and X is walk regular. □

15.3.2 Lemma. *For any graph X we have $\operatorname{tr}(\widehat{M}_X) \geq 1$. If equality holds, then $|V(X)| \leq 2$.*

Proof. Since all multiplicities are integers

$$\sum_r \frac{m_r^2 - m_r}{n} \geq 0$$

and since $\sum_r m_r = n$, it follows that $\operatorname{tr}(\widehat{M}_X) \geq 1$. If equality holds, then $m_r = 1$ for all r and the diagonals of the spectral idempotents are constant, whence X is walk regular. By Theorem 6.3.2 it follows that $n \leq 2$.

15.3.3 Corollary. *If X is a graph on n vertices and $\widehat{M}_X = \frac{1}{n}J$, then $n \leq 2$.* □

15.4 An Ordering

The relation $\succcurlyeq$ is a useful partial ordering on matrices. We briefly investigate some of its properties when applied to average mixing matrices.

15.4.1 Lemma. *Let X and Y be graphs on the same vertex set. If each spectral idempotent of Y is the sum of spectral idempotents of X, then $\widehat{M}_Y \succcurlyeq \widehat{M}_X$.*

Proof. We have

$$(E+F)^{\circ 2} = E^{\circ 2} + F^{\circ 2} + 2E \circ F.$$

If E and F are positive semidefinite, so are the three terms in the sum above, whence

$$(E+F)^{\circ 2} \succcurlyeq E^{\circ 2} + F^{\circ 2}.$$

15.4.2 Lemma. *For any graphs X and Y,*

$$\widehat{M}_{X \square Y} \succcurlyeq \widehat{M}_X \otimes \widehat{M}_Y.$$

Let $E_1, \ldots, E_\ell$ and $F_1, \ldots, F_k$ be the respective spectral idempotents of X and Y. Then each spectral idempotent of $X \square Y$ is a sum of idempotents of the form $E_r \otimes F_s$. To complete the proof, note that

$$(E_r \otimes F_s)^{\circ 2} = E_r^{\circ 2} \otimes F_s^{\circ 2}.$$ □

This lemma will also hold when we use the Laplacian in place of the adjacency matrix. Of course we also have $\widehat{M}_{X\times Y} \succcurlyeq \widehat{M}_X \otimes \widehat{M}_Y$.

If P is a permutation matrix and $A(Y) = P^T A(X) P$, then

$$\widehat{M}_Y = P^T \widehat{M}_X P.$$

This indicates that the partial ordering on average mixing matrices using $\succcurlyeq$ cannot generally correspond to a useful ordering on graphs. Invariants such as $\operatorname{tr}(\widehat{M}_X)$ might be useful or interesting.

15.5 Strongly Cospectral Vertices

15.5.1 Theorem. *Let $\widehat{M}_X$ be the average mixing matrix of the graph X. Then vertices u and v are strongly cospectral if and only if $\widehat{M}_X(e_u - e_v) = 0$.*

Proof. Suppose $N \succcurlyeq 0$ and $N(e_1 - e_2) = 0$. We may assume that the leading 2×2 submatrix of N is

$$\begin{pmatrix} a & b \\ b & d \end{pmatrix}$$

and therefore

$$0 = (e_1 - e_2)^T N (e_1 - e_2) = a + d - 2b.$$

Hence $b = (a+d)/2$. Since $N \succcurlyeq 0$ we have $ad - b^2 \geq 0$ and thus

$$0 \leq 4ad - 4b^2 = 4ad - (a+d)^2 = -(a-d)^2,$$

whence $a = d = b$.

If $\widehat{M}_X(e_u - e_v) = 0$ then

$$0 = (e_u - e_v)^T \widehat{M}_X (e_u - e_v) = \sum_r (e_u - e_v)^T E_r^{\circ 2} (e_u - e_v)$$

and as each summand $E_r^{\circ 2}$ in $\widehat{M}_X$ is positive semidefinite, we have

$$E_r^{\circ 2}(e_u - e_v) = 0$$

for all r. Therefore, for all r,

$$((E_r)_{u,u})^2 = ((E_r)_{u,v})^2 = ((E_r)_{v,v})^2$$

Since

$$(E_r)_{u,v} = \langle E_r e_u, E_r e_v \rangle$$

it follows by Cauchy-Schwarz that $E_r e_u = \pm E_r e_v$. □

One consequence of these results is that, if the rows of the average mixing matrix of X are distinct, there is no perfect state transfer on X.

15.6 Integrality

In investigating the relation between the structure of $\widehat{M}_X$ and the graph X, it can be convenient to scale $\widehat{M}_X$ so that it entries are integers. For this we need to know a common multiple of the denominators of its entries.

15.6.1 Lemma. *If D is the discriminant of the minimal polynomial of A, then $D^2\widehat{M}_X$ is an integer matrix.*

Proof. Let $\theta_1, \ldots, \theta_m$ be the distinct eigenvalues of A. Define polynomials $\ell_r(t)$ by

$$\ell_r(t) := \prod_{s \neq r}(t - \theta_s).$$

We note that $\ell_r(\theta_r) = \psi'(\theta_r)$ and

$$\frac{\ell_r(\theta_s)}{\psi'(\theta_r)} = \delta_{r,s}.$$

Now

$$E_r = \frac{1}{\psi'(\theta_r)}\ell_r(A).$$

The discriminant D of ψ is equal (up to sign) to

$$\prod_{r=1}^{m} \psi'(\theta_r);$$

since the entries of $\ell_r(A)$ are algebraic integers we conclude that the entries of $D^2 E_r^{\circ 2}$ are algebraic integers and therefore the entries of $D^2\widehat{M}_X$ are algebraic integers. Since $\widehat{M}_X$ is rational, the lemma follows. □

We have no reason to believe this lemma is optimal. If the eigenvalues of X are all simple, we can do better.

15.6.2 Theorem. *Let X be a graph with all eigenvalues simple and let D be the discriminant of its characteristic polynomial. Then $D\widehat{M}_X$ is an integer matrix.*

Proof. We have

$$(xI - A)^{-1} = \sum_r \frac{1}{x - \theta_r} E_r$$

and since $(I - tA)^{-1}$ is the walk generating function of X, it follows from the identity stated immediately following Theorem 4.4.3 (or from [35, Corollary 4.1.3]) that

$$(E_r)_{u,v} = \lim_{x \to \theta_r} \frac{(x - \theta_r)\Big(\phi(X \setminus u, x)\phi(X \setminus v, x) - \phi(X \setminus uv, x)\phi(X, x)\Big)^{1/2}}{\phi(X, x)}$$

and since

$$\lim_{x \to \theta_r} \frac{\phi(X, x)}{x - \theta_r} = \phi'(X, \theta_r)$$

we conclude that if θ_r is simple

$$\Big((E_r)_{u,v}\Big)^2 = \frac{\phi(X \setminus u, \theta_r)\, \phi(X \setminus v, \theta_r)}{\phi'(X, \theta_r)^2}.$$

If B is the $n \times n$ matrix with ur-entry $\phi(X \setminus u, \theta_r)$ and Δ is the $n \times n$ diagonal matrix with r-th diagonal entry $\phi'(X, \theta_r)$, it follows that

$$\widehat{M}_X = B \Delta^{-2} B^T.$$

Assume $n = |V(X)|$ and let $\theta_1, \ldots, \theta_n$ be the eigenvalues of X. Let V be the $n \times n$ Vandermonde matrix with ij-entry θ_j^{i-1}. Let ϕ be the characteristic polynomial of X. The discriminant of ϕ is equal to the product of the entries of Δ, we denote it by D.

Let C be the $n \times n$ matrix whose ur-entry is the coefficient of x^{r-1} in $\phi(X \setminus u, x)$. Then $CV = B$ and

$$\widehat{M}_X = CV \Delta^{-2} V^T C^T.$$

Define polynomials $\ell_s(x)$ by

$$\ell_s(x) = \prod_{r \neq s} (x - \theta_r)$$

and let L be the $n \times n$ matrix with sj-entry equal to the coefficient of x^{j-1} in $\ell_s(x)$. Note that

$$\ell_s(\theta_r) = \delta_{r,s} \phi'(\theta_s)$$

and therefore

$$LV = \Delta.$$

Since

$$\Delta = \Delta^T = V^T L^T$$

it follows that

$$\Delta^{-2} = V^{-1} L^{-1} L^{-T} V^{-T}$$

and so

$$V\Delta^{-2}V^T = VV^{-1}L^{-1}L^{-T}V^{-T}V^T = (L^T L)^{-1}.$$

(We're almost done.) The entries of L are algebraic integers. As

$$\det(VV^T) = \det(V)^2 = D$$

and as $LD = \Delta$, we see that $\det(L^T L) = D$. Therefore the entries of

$$D(L^T L)^{-1}$$

are algebraic integers. So the entries of $DV\Delta^{-2}V^T$ are algebraic integers and, since the entries of C are integers, the entries of $D\widehat{M}_X$ are algebraic integers. But the entries of $D\widehat{M}_X$ are rational and therefore they are all integers. □

It is at least plausible that if D is the discriminant of the minimal polynomial of X, then $D\widehat{M}_X$ is an integer matrix.

15.7 Near Enough Implies Strongly Cospectral

We have seen in Sections **??** and 7.2 that if the orbits of e_a under $U(t)$ comes close enough to γe_b (for some γ) then interesting things happen. We offer one more result of the same type.

15.7.1 Lemma. *Let a and b be distinct vertices in the graph X. There is a constant ϵ such that if, for some γ with $|\gamma| = 1$, we have*

$$\|U(t)e_a - \gamma e_b\| < \epsilon,$$

then a and b are strongly cospectral.

Proof. The idea is to show that if $\|U(t)e_a - \gamma e_b\|$ is small enough, the a- and b-rows of $\widehat{M}_X$ are equal.

If

$$U(t)e_a \approx \gamma e_b$$

then

$$e^{it\theta_r} E_r e_a \approx \gamma E_r e_b$$

and consequently for any vertex u of X,

$$(E_r)_{u,b} \approx \gamma^{-1} e^{it\theta_r} (E_r)_{a,b}.$$

Since the entries of E_r are real, this implies that

$$(E_r)^2_{u,b} \approx (E_r)^2_{u,a}$$

and in turn we have

$$(E_r^{\circ}2)e_b \approx (E_r^{\circ 2})e_a.$$

Let D be the discriminant of the minimal polynomial of A. Since the entries of $D^2\widehat{M}_X$ is an integer matrix we conclude that (if ϵ is small enough), then $\widehat{M}_X e_a = \widehat{M}_X e_b$, and therefore a and b are strongly cospectral. □

We leave the task of deriving an explicit expression for ϵ as an exercise. The real problem is to identify examples where we can apply this lemma.

15.8 Average Mixing on Paths

The average mixing matrix for a path has a simpler form then we might expect.

15.8.1 Lemma. *If $E_1, \ldots, E_n$ are the idempotents for P_n, then the average mixing matrix of P_n is*

$$\sum_r E_r \circ E_r = \frac{1}{2n+2}(2J + I + T).$$

Proof. We use 10.2.5:

$$(E_r \circ E_r)_{j,k} = \frac{4}{(n+1)^2} \sin^2\Big(\frac{jr\pi}{n+1}\Big) \sin^2\Big(\frac{kr\pi}{n+1}\Big)$$

which implies that

$$\frac{(n+1)^2}{4}(E_r \circ E_r)_{j,k} = \frac{1}{4}\left(1-\cos\left(\frac{2jr\pi}{n+1}\right)\right)\left(1-\cos\left(\frac{2kr\pi}{n+1}\right)\right).$$

Now

$$\left(1-\cos\left(\frac{2jr\pi}{n+1}\right)\right)\left(1-\cos\left(\frac{2kr\pi}{n+1}\right)\right) =$$
$$1-\cos\left(\frac{2jr\pi}{n+1}\right)-\cos\left(\frac{2kr\pi}{n+1}\right)+\frac{1}{2}\cos\left(\frac{2(j+k)r\pi}{n+1}\right)+\frac{1}{2}\cos\left(\frac{2(j-k)r\pi}{n+1}\right)$$

We need to sum each of the five terms on the right from 1 to n. From 10.2.4 it follows that

$$\begin{aligned}\sum_{r=1}^{n}\cos\left(\frac{2\ell r\pi}{n+1}\right) &= \frac{1}{2}\left(-1+\frac{\sin\left(\frac{(2n+1)\ell\pi}{n+1}\right)}{\sin\left(\frac{\ell\pi}{n+1}\right)}\right)\\ &= \frac{1}{2}\left(-1+\frac{\sin\left(2\ell\pi-\frac{\ell\pi}{n+1}\right)}{\sin\left(\frac{\ell\pi}{n+1}\right)}\right)\\ &= -1.\end{aligned}$$

Consequently

$$\sum_{r=1}^{n}(n+1)^2(E_r \circ E_r)_{j,k} = \begin{cases} 3(n+1)/2, & j=k;\\ 3(n+1)/2, & j+k=n+1\\ n+1, & \text{otherwise}\end{cases}$$

and this completes the proof. □

15.9 Path Laplacians

The average mixing matrix for paths also takes a simple form when we use the Laplacian of a path, rather than its usual adjacency matrix. We employ the notation of 10.5.

15.9.1 Theorem. *The average mixing matrix for the continuous quantum walk using the Laplacian matrix of the path P_n is*

$$\frac{1}{n^2}\left((n-1)J + \frac{n}{2}(I+T)\right).$$

Proof. Set

$$F_r = (2-\theta_r)^{-1} D E_r D^T.$$

Then

$$\begin{aligned}(F_r^{\circ 2})_{j,k} &= \frac{4}{n^2}\cos^2\left(\frac{(2j-1)r\pi}{2n}\right)\cos^2\left(\frac{(2k-1)r\pi}{2n}\right)\\ &= \frac{1}{n^2}\left(1+\cos\left(\frac{(2j-1)r\pi}{n}\right)\right)\left(1+\cos\left(\frac{(2k-1)r\pi}{n}\right)\right)\end{aligned}$$

and

$$\begin{aligned}&\left(1+\cos\Big(\frac{(2j-1)r\pi}{n}\Big)\right)\left(1+\cos\Big(\frac{(2k-1)r\pi}{n}\Big)\right)\\ &\qquad = 1+\cos\Big(\frac{(2j-1)r\pi}{n}\Big)+\cos\Big(\frac{(2k-1)r\pi}{n}\Big)\\ &\qquad\quad + \frac{1}{2}\cos\Big(\frac{(2j+2k-2)r\pi}{n}\Big)+\frac{1}{2}\cos\Big(\frac{(2j-2k)r\pi}{n}\Big).\end{aligned}$$

From 10.2.4 we have

$$\begin{aligned}2\sum_{r=1}^{n-1}\cos\Big(\frac{r\ell\pi}{n}\Big) &= -1+\frac{\sin\Big((n-\frac{1}{2})\frac{\ell\pi}{n}\Big)}{\sin\Big(\frac{\ell\pi}{2n}\Big)}\\ &= -1+\frac{\sin\Big(\ell\pi-\frac{\ell\pi}{2n}\Big)}{\sin\Big(\frac{\ell\pi}{2n}\Big)}\\ &= -1+\frac{-\cos(\ell\pi)\sin\left(\frac{\ell\pi}{2n}\right)}{\sin\left(\frac{\ell\pi}{2n}\right)}\\ &= -((-1)^\ell+1).\end{aligned}$$

It is now easy to derive the stated formula for the average mixing matrix. □

We note that $2I - L(P_n)$ can be viewed as the adjacency matrix of a path on n vertices with a loop of weight one on each end-vertex. Examples show that if we add loops with weight other than 0 or 1, the average mixing matrix is not a linear combination of I, J and T. Thus if we add loops of weight 2 to the end-vertices of P_6, the average mixing matrix is:

$$\frac{1}{2*9*107}\begin{pmatrix} 599 & 218 & 146 & 146 & 218 & 599 \\ 218 & 455 & 290 & 290 & 455 & 218 \\ 146 & 290 & 527 & 527 & 290 & 146 \\ 146 & 290 & 527 & 527 & 290 & 146 \\ 218 & 455 & 290 & 290 & 455 & 218 \\ 599 & 218 & 146 & 146 & 218 & 599 \end{pmatrix}.$$

(Here the discriminant of the characteristic polynomial is $2^6 3^5 107$.)

15.10 Cycles

We determine the average mixing matrices for cycles.

Let P be the permutation matrix corresponding to a cycle of length n and let ζ be a primitive n-th root of unity. Define matrices $F_0, \dots, F_{n-1}$ by

$$(F_r)_{i,j} = \frac{1}{n}\zeta^{r(i-j)}.$$

(Thus the rows and columns of these matrices are indexed by $\{0, \dots, n-1.\}$) Then P is a normal matrix and has the spectral decomposition

$$P = \sum_{r=0}^{n-1} \zeta^r F_r.$$

We also note that

$$F_r \circ F_s = \frac{1}{n} F_{r+s}$$

where the subscripts are viewed as elements of $\mathbb{Z}_n$. The adjacency matrix of the cycle on n vertices is $P + P^T$. Define E_0 to be F_0 and, if $0 < r < n/2$, we set

$$E_r = F_r + F_{n-r}.$$

Further $E_0 := F_0$ and, if n is even then $E_{n/2} := F_{n/2}$. Then if n is odd,

$$E_0, \dots, E_{(n-1)/2}$$

are the idempotents in the spectral decomposition of $A(C_n)$ and the corresponding eigenvalues are

$$\theta_r = \zeta^r + \zeta^{-r}, \qquad r = 0, \dots, \frac{n-1}{2};$$

if n is even we have the additional idempotent $E_{n/2}$ with eigenvalue $\zeta^{n/2} = -1$.

15.10.1 Lemma. *If n is odd then the average mixing matrix of the cycle C_n is*

$$\frac{n-1}{n^2}J + \frac{1}{n}I,$$

if n is even it is

$$\frac{n-2}{n^2}J + \frac{1}{n}(I + P^{n/2}).$$

Proof. Assume first that $n = 2m+1$. Then the average mixing matrix is

$$\begin{aligned}\sum_{r=0}^{m} E_r^{\circ 2} &= F_0^{\circ 2} + \sum_{r=1}^{m}(F_r + F_{-r})^{\circ 2}\\ &= \frac{1}{n}F_0 + \frac{1}{n}\sum_{r=1}^{m}(F_{2r} + F_{-2r} + 2F_0)\\ &= F_0 + \frac{1}{n}\sum_{r=1}^{n-1}F_r\\ &= \frac{1}{n}I + \frac{n-1}{n}F_0.\end{aligned}$$

Now suppose $n = 2m$. Then the average mixing matrix is

$$\begin{aligned}E_m^{\circ 2} + \sum_{r=0}^{m-1} E_r^{\circ 2} &= F_0^{\circ 2} + F_m^{\circ 2} + \sum_{r=1}^{m-1}(F_r + F_{-r})^{\circ 2}\\ &= \frac{1}{n}F_0 + \frac{1}{n}F_0 + \frac{1}{n}\sum_{r=1}^{m-1}(F_{2r} + F_{-2r} + 2F_0)\\ &= F_0 + \frac{1}{n}\sum_{r=1}^{m-1}(F_{2r} + F_{-2r})\\ &= \frac{n-2}{n}F_0 + \frac{2}{n}\sum_{r=0}^{m-1}F_{2r}.\end{aligned}$$

Since

$$P^m F_s = (\zeta^m)^s F_s = (-1)^s F_s$$

we see that P^m has spectral decomposition

$$P^m = \sum_{s=0}^{n-1} (-1)^s F_s$$

and consequently

$$\frac{1}{2}(I + P^m) = \sum_{r=0}^{m-1} F_{2r}.$$

Our stated formula for the average mixing matrix follows. □

In general the average mixing matrix for a circulant can be more complex in structure than the average mixing matrix of a cycle. We will see in the next section that graphs in pseudocyclic schemes provide the right generalization of cycles or, at least, of odd cycles.

It is easy for different circulants of order n to have the same spectral idempotents, any two such circulants necessarily have the same average mixing matrix.

15.11 Average Mixing on Pseudocyclic Graphs

An association scheme is *pseudocyclic* if the multiplicities $m_1, \ldots, m_d$ are equal (in which case their common value is $(v-1)/d$). If a scheme is pseudocyclic then $v_1, \ldots, v_d$ are necessarily all equal to $(v-1)/d$. For details see Brouwer, Cohen and Neumaier[14, §2.2B].

We note one class of examples, the *cyclotomic schemes*. Assume q is a prime power and d divides $q-1$. Let $\mathbb{F}$ be the finite field of order q and let S be the subgroup of the multiplicative group of $\mathbb{F}$ generated by the non-zero d-th powers. Thus $|S| = (q-1)/d$. Let $S_1, \ldots, S_d$ denote the cosets of S in $\mathbb{F}^*$, with $S_1 = S$. Now we define the matrices of an association scheme with d classes and with vertex set $\mathbb{F}$ by setting $A_0 = I$ and

$$(A_i)_{x,y} = 1, \qquad (i = 1, \ldots, d)$$

if and only if $y - x$ is in S_i. These matrices form the cyclotomic scheme with d classes on $\mathbb{F}$. It is symmetric if and only if $-1 \in S$. The directed graphs $X_1, \ldots, X_d$ such that $A_i = A(X_i)$ are all isomorphic. The most well known case is when $d = 2$ and $q \cong 1$ modulo four, in which case the two graphs we have constructed are the *Paley graphs*.

We note that there are pseudocyclic schemes which are not cyclotomic, and that there are pseudocyclic schemes with two classes where the two graphs are asymmetric, that is, their only automorphism is the identity.

15.11.1 Theorem. *Suppose X is a graph in a d-class pseudocyclic scheme on n vertices consisting of graphs of valency $m = (n-1)/d$. Then the average mixing matrix of X is*

$$\frac{n-m+1}{n^2}J + \frac{m-1}{n}I.$$

Proof. Koppinen [46] proved that for an association scheme with d classes we have

$$\sum_{i=0}^{d} \frac{1}{nv_i} A_i \otimes A_i^T = \sum_{j=0}^{d} \frac{1}{m_j} E_j \otimes E_j.$$

If the scheme is symmetric then $A_i \circ A_i = A_i$ and, since $M \circ N$ is a submatrix of $M \otimes N$, Koppinen's identity yields that

$$\sum_{i=0}^{d} \frac{1}{nv_i} A_i = \sum_{j=0}^{d} \frac{1}{m_j} E_j \circ E_j.$$

For any scheme, we have $m_0 = v_0 = 1$ and for a pseudocyclic scheme

$$m_i = v_i = \frac{n-1}{d}, \quad i = 1, \ldots, d.$$

As $\sum_i A_i = J$ and $\sum_j E_j = I$, if $m = (n-1)/d$ we find that

$$\frac{1}{n}\Big(I + \frac{1}{m}(J - I)\Big) = \frac{1}{n^2}J + \frac{1}{m}\sum_{j=1}^{d} E_j^{\circ 2}\Big)$$

and hence

$$\frac{1}{m}\sum_{j=1}^{d} E_j^{\circ 2} = \left(\frac{1}{nm} - \frac{1}{n^2}\right) J + \frac{m-1}{nm} I = \frac{n^2 - nm}{n^3 m} J + \frac{m-1}{nm} I. \qquad \square$$

A graph in a pseudocyclic scheme with two classes is known as a *conference graph*, and there are examples whose automorphism group is trivial.

15.12 Average Mixing on Oriented Graphs

If the average mixing matrix of the continuous quantum walk relative to the adjacency matrix of a graph X is $\frac{1}{n}J$, then $|V(X)| \le 2$. For oriented adjacency matrices the situation is more interesting.

15.12.1 Theorem. *If all vertices in the oriented graph X are strongly cospectral, the average mixing matrix for the quantum walk on X is $\frac{1}{n}J$.*

Proof. If $U(t) = \sum_r e^{t\theta_r} E_r$ then

$$\overline{U(t)} = \sum_r e^{-t\theta_r} \overline{E_r}$$

and hence the mixing matrix for the quantum walk based on A is

$$U(t) \circ \overline{U(t)} = \sum_r E_r \circ \overline{E_r} + \sum_{r \neq s} e^{t(\theta_r - \theta_s)} E_r \circ \overline{E_s}.$$

It follows that the average mixing matrix $\widehat{M}_X$ is given by

$$\widehat{M}_X = \sum_r E_r \circ \overline{E_r} = \sum_r E_r \circ E_r^T.$$

If the eigenvalue θ_r is simple and z is an eigenvector for it with norm 1, then $E_r = zz^T$ and consequently

$$E_r \circ \overline{E_r} = zz^* \circ \bar{z}z^T = (z \circ \bar{z})(\bar{z} \circ z)^T.$$

If z is flat then $z \circ \bar{z} = \frac{1}{n}\mathbf{1}$ and $E_r \circ \overline{E_r} = \frac{1}{n^2}\mathbf{1}$. □

15.12.2 Lemma. *Vertices a and b in an oriented graph are strongly cospectral if and only if $\widehat{M}_X e_a = \widehat{M}_X e_b$.*

Proof. If E is positive semidefinite then so is $\overline{E}$; hence $E \otimes \overline{E}$ is positive semidefinite and therefore its principal submatrix $E \circ \overline{E}$ is positive semidefinite. Hence $\widehat{M}_X \succcurlyeq 0$ and therefore $\widehat{M}_X(e_a - e_b) = 0$ if and only if $(e_a - e_b)^T \widehat{M}_X (e_a - e_b) = 0$. Since the matrices $E_r \circ \overline{E_r}$ are positive semidefinite, we see that $\widehat{M}_X(e_a - e_b) = 0$ if and only if $(E_r \circ \overline{E_r})(e_a - e_b) = 0$. Now

$$e_u^T (E_r \circ \overline{E_r})(e_a - e_b) = |(E_r)_{u,a}|^2 - |(E_r)_{u,b}|^2$$

and so if $(E_r \circ \overline{E_r})(e_a - e_b) = 0$, then

$$|(E_r)_{a,a}|^2 = |(E_r)_{a,b}|^2 = |(E_r)_{b,b}|^2$$

for all r. Therefore by Cauchy-Schwarz, the vectors $E_r e_a$ and $E_r e_b$ are parallel. Since $|(E_r)_{a,a}|^2 = |(E_r)_{b,b}|^2$ for all r, the vertices a and b are cospectral. □

If the triangle bound is tight, then there is a complex number γ of norm 1 such that

$$\gamma = e^{it\theta_r} \frac{(E_r)_{a,b}}{|(E_r)_{a,b}|}$$

for all r such that $(E_r)_{a,b} \neq 0$. Since I have nothing useful to say about the ratios that appear here, I have not been able to deduce any useful consequences.

15.13 Average States

Suppose D is density matrix with rows and columns indexed by $V(X)$. We define

$$D(t) = U(t)DU(-t)$$

and

$$\Psi(D) = \lim_{T\to\infty} \frac{1}{T} \int_0^T D(t)\,dt.$$

We say that $\Psi(D)$ is the *average* of the state D. As

$$D(t) = \sum_{r,s} e^{it(\theta_r - \theta_s)} E_r D E_s,$$

it follows that

$$\Psi(D) = \sum_r E_r D E_r.$$

You should note that $\Psi(D) \succcurlyeq 0$ and you should verify that $\operatorname{tr}(\Psi(D)) = \operatorname{tr}(D)$, whence an average state is a density matrix. Before developing the theory of average states, we note the connection with average mixing. Recall that if $a \in V(X)$, then

$$D_a = e_a e_a^T.$$

15.13.1 Theorem. *The average mixing matrix of X is the Gram matrix of the vertex states D_a for a in $V(X)$.*

The *commutant* of a set of matrices S is the set of matrices that commute with each element of S. We denote it by $\operatorname{comm}(S)$, and note that it is a matrix algebra.

15.13.2 Theorem. *If D is the density matrix of a state on $V(X)$, then $\Psi(D)$ is the orthogonal projection of D onto $\operatorname{comm}(A)$.*

Proof. Any matrix of the form $E_r M E_r$ commutes with A, and therefore $\Psi(M)$ lies in $\operatorname{comm}(A)$. It is also immediate that $\Psi^2(M) = \Psi(M)$. If $N \in \operatorname{comm}(A)$, then N commutes with each spectral idempotent E_r and therefore $\Psi(N) = N$. Thus we have shown that Ψ is an idempotent linear map with image $\operatorname{comm}(A)$. To prove that it is an orthogonal projection we must show that it is self-adjoint:

$$\langle M, \Psi(N)\rangle = \sum_r \operatorname{tr}(M E_r N E_r) = \sum_r \operatorname{tr}(E_r M E_r N) = \langle \Psi(M), N\rangle. \qquad \square$$

15.13.3 Lemma. *Suppose $E_1, \ldots, E_m$ are the spectral idempotents of A. If $D = zz^*$ is a pure state, then the eigenvalues of $\Psi(D)$ are $z^* E_r z$ for $r = 1, \ldots, m$.*

Proof. Suppose $D = zz^*$ is a pure state. Then

$$(E_r D E_r)^2 = E_r zz^* E_r zz^* E_r = (z^* E_r z) E_r zz^* E_r$$

which shows that

$$(z^* E_r z)^{-1} E_r zz^* E_r$$

is an idempotent. Therefore we have the spectral decomposition

$$\Psi(D) = \sum_r z^* E_r z \left((z^* E_r z)^{-1} E_r zz^* E_r\right),$$

and this leads to the stated expressions for the eigenvalues of $\Psi(D)$. $\square$

It follows that the eigenvalues of $\Psi(D_a)$ are the spectral density of the vertex a, The entropy of the spectral density of a is the von Neumann entropy of $\Psi(D_a)$.

We have another characterization of strongly cospectral vertices.

15.13.4 Lemma. *Two vertices a and b are strongly cospectral if and only if $\Psi(D_a) = \Psi(D_b)$.*

Notes

Exercises

Chapter 16

Translation Graphs

If there is perfect state transfer between two vertices in a graph, they must be similar in some fairly strong sense. Vertex-transitive graphs provide a class of graphs where any two vertices are equivalent under the automorphism group, and so it is natural to look for perfect state transfer in this class. In this chapter we restrict ourselves further by focussing on Cayley graphs for abelian groups. The advantage of this class of graphs is that we can readily determine their eigenvalues and eigenvectors using the character theory of the underlying group.

In dealing with vertex-transitive graphs, we view each edge *ab* as a pair of arcs (a, b) and (b, a). The *Cayley graph* $X(G, \mathcal{C})$ has the group G as its vertex set, and the pair of vertices (x, y) is an arc if $yx^{-1} \in \mathcal{C}$. A *translation graph* is a Cayley graph for an abelian group. If $1 \in \mathcal{C}$ than we get a loop on each vertex; we will usually assume $1 \notin C$ and thereby avoid this. To ensure we get a graph (rather than a directed graph) if and only $C = C^{-1}$, that is, if $x \in C$ then $x^{-1} \in \mathcal{C}$. In this case we say $\mathcal{C}$ is *inverse-closed*.

16.1 Strongly Cospectral Vertices in Vertex-Transitive Graphs

Some of the results we need are proved just as easily for vertex-transitive graphs as for translation graphs, so in this section we work in the more general setting.

strong-cosp is aut-invariant equivalence relation strong-cosp -> order-two symmetry (cite) strong-cosp + vx transitive -> central order two autom strong-cosp + Cayley for G -> autom is in G

16.2 Strongly Cospectral Vertices in Translation Graphs

Let G be an abelian group of order n. As ψ runs over the characters of G, the $n \times n$ matrices E_ψ defined by

$$(E_\psi)_{g,h} = \frac{1}{n}\psi(hg^{-1}).$$

are the primitive spectral idempotents of the group scheme of G. If $X = X(G, \mathcal{C})$, then it follows that

$$A = \sum_{\psi} \psi(\mathcal{C}) E_\psi;$$

this is a refinement of the spectral decomposition of A.

16.2.1 Lemma. *The vertices* 0 *and* c *are strongly cospectral vertices in* $X(G, \mathcal{C})$ *if and only if* $2c = 0$ *and for any two characters* φ *and* ψ, *if* $\varphi(\mathcal{C}) = \psi(\mathcal{C})$ *then* $\varphi(c) = \psi(c)$.

Proof. For each eigenvalue θ of X, let $P(\theta)$ denote the set of characters ψ such that $\psi(\mathcal{C}) = \theta$. If E represents projection onto the θ-eigenspace, then

$$E = \sum_{\psi \in P(\theta)} E_\psi$$

and therefore

$$E_{0,c} = \sum_{\psi \in P(\theta)} (E_\psi)_{0,c} = \frac{1}{n} \sum_{\psi \in P(\theta)} \psi(c).$$

Since $E_{0,0} = |P(\theta)|/n$, we conclude that $|E_{0,c}| = E_{0,0}$ if and only all characters in $P(\theta)$ take the same value, γ say, on c. But since the eigenvalues of X are real, E is symmetric, and therefore $|E_{0,-c}| = E_{0,0}$. This implies that $\psi(-c) = \gamma$ for all characters in $P(\theta)$. As $\psi(c)\psi(-c) = \psi(0) = 1$, we find that $\gamma = \pm 1$.

If 0 and c are strongly cospectral, then $\psi(c) = \pm 1$ for every character of G and therefore $2c = 0$. □

16.3 State Transfer on Translation Graphs

Using Theorem **??**, we obtain the following.

16.3.1 Lemma. *Let δ be the greatest common divisor of the eigenvalue differences of the translation graph $X = X(G, \mathcal{C})$. If perfect state transfer occurs on X, it occurs at time π/δ.* □

We now characterize when perfect state transfer takes place on a translation graph.

16.3.2 Lemma. *Let G be an abelian group, let $X = X(G, \mathcal{C})$ be a Cayley graph for G with integer eigenvalues, and let δ be the gcd of the difference of the eigenvalues of X. We have perfect state transfer from 0 to c on X at time π/δ if and only if, for each character ψ of G,*

$$\psi(c) = (-1)^{(|\mathcal{C}|-\psi(\mathcal{C}))/\delta}.$$

Proof. We have

$$U(t)_{0,c} = \sum_{\psi} e^{it\psi(\mathcal{C})}(E_\psi)_{0,c} = \frac{1}{n}\sum_{\psi} e^{it\psi(\mathcal{C})}\overline{\psi(0)}\psi(c) = \frac{1}{n}\sum_{\psi} e^{it\psi(\mathcal{C})}\psi(c).$$

Since all summands have absolute value 1, we see that $|U(t)_{0,c}| = 1$ if and only if all summands have the same phase, that is, if and only if they are all equal. This means that

$$e^{it|\mathcal{C}|} = e^{it\psi(\mathcal{C})}\psi(c)$$

for all characters ψ. □

16.4 Sums and Complements

Suppose $X = X(G, \mathcal{C})$ where $\mathcal{C}$ is the disjoint union of inverse-closed subsets $\mathcal{C}_1$ and $\mathcal{C}_2$. Then

$$A(X) = A(X(G, \mathcal{C}_1)) + A(X(G, \mathcal{C}_2)),$$

equivalently the edge set of X is the disjoint union of the edge sets of two smaller Cayley graphs, each spanning subgraphs of X. It will be difficult to make use of this decomposition unless the adjacency matrices of these subgraphs commute. If G is abelian, this is not an issue.

16.4.1 Lemma. *Let $\mathcal{C}$ be an inverse-closed subset of the abelian group G with a partition into inverse-closed subsets $\mathcal{C}_1$ and $\mathcal{C}_2$. If $X(\mathcal{C}_1)$ admits perfect state transfer at time τ and $X(\mathcal{C}_2)$ is periodic with period τ, then $X(\mathcal{C})$ admits perfect state transfer at time τ.* □

Any graph X together with its complement, determines a partition of $E(K_n)$ and

$$A(K_n) = A(X) + nA(\overline{X}).$$

Here $A(X)$ and $A(\overline{X})$ commute if and only if X is regular. The complete graph K_n is periodic, with period $2\pi/n$. If X is regular then

$$U_{\overline{X}}(t) = U_{K_n}(t)U_X(-t)$$

and so we can relate properties of the continuous walk on $\overline{X}$ to those of the walk on X.

By way of example, consider the cocktail party graph $\overline{mK_2}$. The eigenvalues of $\overline{mK_2}$ are

$$2m-2,\ 0,\ -2,$$

so the gcd of its eigenvalue differences is two and this graph is periodic with period π. Hence if perfect state transfer occurs, it occurs at time $\pi/2$. Now

$$U_{K_n}(\pi/2) = e^{-\pi i/2}(e^{\frac{1}{2}n\pi i}E_0 + E_1)$$

and

$$U_{mK_2}(\pi/2) = iA(mK_2);$$

given this it is an easy exercise now to show that we have perfect state transfer on $\overline{mK_2}$ if and only if m is even.

16.5 Integral Translation Graphs

There is a convenient characterization of the translation graphs with only integer eigenvalues. Define elements g and h in the abelian group G to be *equivalent* if $\langle g\rangle = \langle h\rangle$, i.e., g and h generate the same cyclic subgroup of G. We denote this equivalence relation by $g \approx h$. Bridges and Mena [] proved the following result.

16.5.1 Lemma. *Let G be an abelian group. The eigenvalues of the Cayley graph $X(G,\mathcal{C})$ are all integers if and only if $\mathcal{C}$ is $\mathcal{C}$ is the union of $\approx$-classes.* □

We note two special cases. If p is a prime, it follows that the only Cayley graphs for $\mathbb{Z}_p$ will all eigenvalues integer are K_p and the empty graphs $\overline{K}_n$. On the other hand, if $G = \mathbb{Z}_2^d$, all Cayley graphs for G have only integer eigenvalues. This holds for $\mathbb{Z}_3^d$, $\mathbb{Z}_4^d$ and $\mathbb{Z}_6^d$, and for all linear graphs as well. (As you may prove.)

Suppose G is abelian of order n and $\mathcal{C}$ is a connection set for a Cayley graph for G. If h is an element of $\mathcal{C}$ with order two, then $X(G, \{h\})$ is a spanning subgraph of X isomorphic to a perfect matching with $n/2$ edges. If the order $|h|$ of h is k and $k > 2$, then $X(G, \{h, h^{-1})$ is a spanning subgraph of X isomorphic to the disjoint union of n/k cycles C_k. Thus X has a natural expression as the edge-disjoint union perfect matchings and subgraphs $(n/k)C_k$.

Our concern is with integral translation graphs, where the connection set $\mathcal{C}$ is partitioned into equivalence classes for $\approx$, and so we consider the structure of these graphs. Thus we want to describe the graphs of the form $X(G, [g])$, where $g \in G$. If $|g| = m$, then $X(G, [g])$ consists of n/m vertex-disjoint copies of the circulant $X(\mathbb{Z}_m, [g])$. Here g is a generator of $\mathbb{Z}_m$, and therefore $X(\mathbb{Z}_m, [g]) \cong X(\mathbb{Z}_m, [1])$.

The next two results depend on properties of the group of units in the ring $\mathbb{Z}_n$. The details are summarized in Section **??**.

16.5.2 Lemma. *If q is the largest power of the prime p that divides m, then*

$$X(\mathbb{Z}_m, [1]) \cong X(\mathbb{Z}_q, [1]) \times X(\mathbb{Z}_{m/q}, [1]). \qquad \square$$

16.5.3 Lemma. *If q is a power of the prime p, then*

$$X(\mathbb{Z}_q, [1]) \cong \overline{pK_{q/p}}. \qquad \square$$

Combining these two lemmas, we get the following.

16.5.4 Lemma. *Suppose G is abelian with cyclic Sylow 2-subgroup and $X = X(G, \mathcal{C})$ is integral. Let H be the subgroup of G generated by the elements of odd order and let $\mathcal{C}_k$ denote the subset of $\mathcal{C}$ consisting of the elements in $\mathcal{C}$ with order 2^k times an odd number. Then X is the edge-disjoint union of the graphs $X(G, \mathcal{C}_k)$ and, if $k \geq 1$ there is a Cayley graph Y_k of H such that*

$$X(G, \mathcal{C}_k) \cong K_{2^{k-1}, 2^{k-1}} \times Y_k.$$

The Cayley graphs Y_k may have loops. $\square$

16.6 State Transfer on Translation Graphs with $4k+2$ Vertices

We begin with an application of the theory of association schemes.

16.6.1 Lemma. *If G is an abelian group of odd order, then any non-empty integral Cayley graph for G has an odd eigenvalue.*

Proof. Let P be the matrix of eigenvalues of the integral group scheme of G. Assume $n = |G|$ and that this scheme has d classes. Now recall Equation (14.6.1):

$$P\Delta_m P^* = n\Delta_v.$$

Since the eigenvalues are integers and since $\Delta_v = \Delta_m$ (by our remarks at the end of Section 14.8), we thus have

$$\det(P)^2 = n^{d+1}$$

and therefore $\det(P)$ is odd. If x is 01-vector of length d, then the entries of Px are the eigenvalues of the matrix

$$\sum_{i \in \text{supp}(x)} A_i.$$

If the entries of Px are even, then $Px \cong 0$ modulo 2, but P is invertible modulo 2 and therefore x is zero modulo 2. □

Translation graphs of odd order cannot admit perfect state transfer. The perfect matching mK_2 admits perfect state transfer at time $\pi/2$; here we show that if X is a translation graph on n vertices $n \equiv 2$ modulo 4, then X admits perfect state transfer if and only if it is isomorphic to mK_2.

16.6.2 Theorem. *Suppose G is an abelian group of order $2m$, where m is odd and let X be a Cayley graph for G. If X admits perfect state transfer, then $X \cong mK_2$ and perfect state transfer occurs at time $\pi/2$.*

Proof. Let H be the unique subgroup of index two in G, and note that $|H|$ is odd. Assume $X = X(G, \mathcal{C})$. Set $\mathcal{C}_0 = \mathcal{C} \cap H$ and $\mathcal{C}_1 = \mathcal{C} \setminus H$. (This is consistent with the usage in Lemma 16.5.4.) There are Cayley graphs Y_0 and Y_1 for H, with respective adjacency matrices A_0 and A_1, such that

$$A(X) = \begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix}.$$

Thus in the notation from Section 12.7, we have that $X \cong Y_0 \oslash Y_1$. If X admits perfect state transfer, then it admits perfect state transfer from 0 to the unique element, σ say, with order two in G. Clearly $\sigma \notin H$, and so either case (a) or case (c) of Theorem 12.7.1 applies—that is, either $A + B$ and $A - B$ are periodic at time t with respective phase factors λ and $-\lambda$, or these matrices admit perfect state transfer at time t with respective phase factors λ and $-\lambda$. Since m is odd though, we cannot have perfect state transfer and so (c) is irrelevant.

In case (a), if

$$U_{A_0+A_1}(t) = \lambda I, \quad U_{A_0-A_1}(t) = -\lambda I,$$

then

$$U_{2A_1}(t) = U_{A_0+A_1}(t)\, U_{A_1-A_0}(t) = U_{A_0+A_1}(t)\, \overline{U_{A_0-A_1}(t)} = -I.$$

If $\beta_1, \ldots, \beta_d$ denote the eigenvalues of A_1, then for $r = 1, \ldots, d$ we have

$$e^{2it\beta_r} = -1$$

and therefore there are integers m_r such that

$$2t\beta_r = (2m_r + 1)\pi.$$

Hence the ratios β_r/β_s must all be odd.

The valency of a Cayley graph for a group of odd order is even. If the group is also abelian and the Cayley graph is connected, then by the previous lemma it also has an odd eigenvalue. If we allow a loop on each vertex, then we still have eigenvalues of different parity. We conclude that Y_1 must be the empty graph and $A_1 = I$. If Y_0 is not empty then X is the Cartesian product $Y_0 \,\square\, K_2$. To complete the proof, we show that if Y is not empty, perfect state transfer does not occur on $Y_0 \,\square\, K_2$.

Assume by way of contradiction that we have perfect state transfer at time t, so

$$U_{Y \square K_2}(t) = \gamma R$$

where R is a permutation matrix with zero diagonal of order two. The LHS here is equal to $U_{Y_0}(t) \otimes U_{K_2}(t)$ and so both $U_{Y_0}(t)$ and $U_{K_2}(t)$ must be scalar multiples of permutation matrices. Since $|V(Y_0)|$ is odd, perfect state transfer does not occur on Y and therefore $U_{Y_0}(t)$ must be a multiple of I. If $S = A(nK_2)$ then

$$U_{K_2}(t) = \cos(t)I + i\sin(t)S$$

and therefore $t = (2m+1)\pi/2$ for some integer m. If $\theta_1, \ldots, \theta_n$ are the eigenvalues of Y_0, the eigenvalues of $U_{Y_0}(t)$ are

$$e^{i\pi(2m+1)\theta_r/2}, \quad r = 1, \ldots, n.$$

If θ_r is odd, the corresponding eigenvalue of $U_{Y_0}(t)$ is $\pm i$, if it is even then the eigenvalue is ± 1. Since Y_0 has both positive and negative eigenvalues, we conclude that $U_Y(t)$ is not a scalar multiple of I.

Finally if Y_0 is empty, then $X = nK_2$, which has perfect state transfer at $\pi/2$. □

16.7 Cyclic Sylow 2-Subgroups

In a series of three papers [8, 9, 7], Bašić and others characterized the circulants that admit perfect state transfer. Here we will consider the more general problem of characterizing the graphs with perfect state transfer that are Cayley graphs for abelian groups with cyclic Sylow 2-subgroup. One consequence of their results is that if a circulant graph admits perfect state transfer, it admits perfect state transfer at time $\pi/2$. We present a proof of this for a somewhat larger class of graphs.

We consider perfect state transfer on Cayley graphs for abelian groups with a cyclic Sylow 2-subgroup, equivalently abelian groups with a unique element of order two. Assume $|G| = 2^d m$, where m is odd, and suppose $X = X(G, \mathcal{C})$. As in Lemma 16.5.4, let H be the subgroup of G generated by its elements of odd order and let $\mathcal{C}_k$ denote the subset of $\mathcal{C}$ formed by those elements with order 2^k times an odd number. As before, we have Cayley graphs $Y_0, \ldots, Y_d$ for H. Denote their adjacency matrices by $A_0, \ldots, A_d$.

If $B_0, \ldots, B_k$ are $m \times m$ matrices define $2^k m \times 2^k m$ matrices $\mathcal{M}(A_0, \ldots, A_k)$ recursively by

$$\mathcal{M}(B_0, B_1) = \begin{pmatrix} B_0 & B_1 \\ B_1 & B_) \end{pmatrix}$$

when $r = 1$ and, if $r \geq 2$,

$$\mathcal{M}(B_0, \ldots, B_r) = I_2 \otimes \mathcal{M}(B_0, \ldots, B_{r-1}) + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes (J_{2^{r-1}} \otimes B_r).$$

Thus the adjacency matrix for $X(G,\mathcal{C})$ is $\mathcal{M}(A_0,\ldots,A_k)$.

A *signed Cayley graph* is a Cayley graph together with a function from its connection set $\mathcal{C}$ to $\{\pm 1\}$. If $\mathcal{C}_0$ is the subset of elements of $\mathcal{C}$ with postive sign and $\mathcal{C}_1$ is the subset with negative sign, then the signed adjacency matrix of $X(G,\mathcal{C})$ is $A_0 - A_1$, where $A_i = A(X(G,\mathcal{C}_i))$. The results of the previous section apply without change to signed Cayley graphs.

16.7.1 Theorem. *Let G be an abelian group with cyclic Sylow 2-subgroup. If perfect state transfer occurs on G, it occurs at time $\pi/2$.*

Proof. We employ the notation given above. Assume $|G|$ is divisible by four. If we have perfect state transfer on G, then we have perfect state transfer on G from 0 to the unique element of order two in G, which lies in the subgroup of G generated by $\mathcal{C}_0 \cup \mathcal{C}_1$. Hence Theorem 12.7.1(b) applies: if $r \geq 2$ and we have perfect state transfer on the graph with adjacency matrix $\mathcal{M}(A_0,\ldots,A_r)$ at time t with phase γ, we have perfect state transfer at time t on

$$\mathcal{M}(A_0 - A_r, A_1 - A_r, \ldots, A_{r-1} - A_r).$$

Accordingly we have perfect state transfer at time t on $\mathcal{M}(A_0 - A_2, A_1 - A_2)$ at time t. This matrix is the signed adjacency matrix of a Cayley graph for an abelian group of order $2m$ and so, by Theorem 16.6.2, if it admits perfect state transfer then it admits perfect state transfer at time $\pi/2$. $\square$

Suppose G is abelian of order $2^k m$, where m is odd, and let H be the subgroup of G of order m. If $X = X(G,\mathcal{C})$, define $\mathcal{C}_r$ to be the subset of elements of $\mathcal{C}$ with order 2^r times an odd number. By Lemma 16.5.4 we have that X is the edge-disjoint union of the Cayley graphs $X(G,\mathcal{C}_k)$ for $r = 0,\ldots,k$, where $X(G,\mathcal{C}_k) \cong K_{2^{k-1},2^{k-1}} \times Y_k$ and Y_k is a Cayley graph for H.

Suppose we have perfect state transfer on X at time $\pi/2$. Since the eigenvalues of $K_{2^{k-1},2^{k-1}}$ are 0 and $\pm 2^{k-1}$, the graphs $K_{2^{k-1},2^{k-1}} \times Y_k$ for $k \geq 3$ are all periodic at time $\pi/2$.

16.7.2 Corollary. *Suppose G is abelian of order $2^k m$ where m is odd, let G_2 denote the subgroup of G with order m and assume that the Sylow 2-subgroup of G is cyclic. Then the Cayley graph $X(G,\mathcal{C})$ admits perfect state transfer if and only if $X(G_2,\mathcal{C} \cap G_2)$ admits perfect state transfer.*

16.8 Linear Graphs

The results in this section could well be called folklore.

The additive group of a vector space V over $\mathbb{F}$ is an abelian group, and if the characteristic of $\mathbb{F}$ is p, then it is an elementary abelian p-group. Suppose G is the additive group of V and X is the Cayley graph $X(G, C)$. We say that X is *linear* over $\mathbb{F}$ if C is closed under multiplication by non-zero elements of $\mathbb{F}$; if $\dim(V) = d$ we will say that X has dimension d.

Our goal here is to derive an explicit form for the eigenvalues of a linear graph. One consequence of this that the eigenvalues are integers.

For linear Cayley graphs of dimension d we can represent the connection set by a $d \times m$ matrix M such that no column is a scalar multiple of another. Two elements of $\mathbb{F}^d$ will be adjacent if their difference is non-zero scalar multiple of a column of M. Hence the valency of X is $(|\mathbb{F}| - 1)m$. We will view M as the generator matrix of a code, and then our condition on the columns of M can be restated as the requirement that the minimum distance of the dual code is at least three. We do not insist that the rows of M be linearly independent, although that will be the most interesting case. The *weight* $\mathrm{wt}(x)$ of a vector is the number of non-zero entries in it.

Assume $\mathbb{F}$ has characteristic p and let ζ be a primitive p-th root of 1. If $a \in V = V(n, \mathbb{F})$, the map ψ_a given by

$$\psi_a(x) := \zeta^{\mathrm{tr}(a^T x)}$$

is a character on V. Now

$$\sum_{\beta \in \mathbb{F} \setminus 0} \psi_a(\beta x) = \sum_{\beta \in \mathbb{F} \setminus 0} \zeta^{\mathrm{tr}(\beta a^T x)}$$

This leads us to two cases. If $a^T x = 0$ then the sum is equal to $|\mathbb{F}| - 1$. If $a^T x \neq 0$ then, as β runs over $\mathbb{F} \setminus 0$, the product $\beta a^T x$ runs over all elements of $\mathbb{F} \setminus 0$. Since the trace map is not zero it is onto, and consequently when β runs over $\mathbb{F}$ then the quantity $\mathrm{tr}(\beta a^T x)$ assumes each possible value in $GF(p)$ the same number of times. Now

$$\sum_{\alpha \in \mathbb{F}} \zeta^{\mathrm{tr}(\alpha)} = \frac{|\mathbb{F}|}{p} \sum_{r=0}^{p-1} \zeta^r = 0$$

and it follows that if $a^T x \neq 0$, our sum is equal to -1.

16.8.1 Theorem. *Let $\mathbb{F}$ be a finite field of order q and let ζ be a primitive p-th root of 1 in $\mathbb{C}$. Let M be a $d \times m$ matrix over $\mathbb{F}$ such that no column is a scalar multiple of another, and let $X(M)$ be the associated linear Cayley graph of dimension d. If $a \in \mathbb{F}$ and $\psi_a(x) := \zeta^{\mathrm{tr}(a^T x)}$, then the eigenvalue belonging to ψ_a is $(q-1)m - q\,\mathrm{wt}(a^T M)$.*

Proof. When we sum ψ_a over the connection set, each column of M contributes $q-1$ it it lies in $\ker(a^T)$ and -1 if it does not. As $(a^T M)_r = 0$ if and only if the r-th column of M lies in $\ker(a^T)$, the eigenvalue of ψ_a is

$$(q-1)(m - \mathrm{wt}(a^T M)) + (-1)\,\mathrm{wt}(a^T M) = (q-1)m - q\,\mathrm{wt}(a^T M). \qquad \square$$

The row space of M is a *linear code* over $\mathbb{F}$. The number of columns of M is the length of the code. The code is *projective* if no two columns are linearly dependent or, equivalently, if the minimum distance of the dual is at least three. If a_r denotes the number of code words of weight r in our code, the sequence

$$(a_0, \dots, a_n)$$

is the *weight distribution* of the code. If C is a projective code of length n over a field of order q then, by 16.8.1, the integer

$$(q-1)n - qr$$

is an eigenvalue of $X(C)$ with multiplicity a_r. Thus the eigenvalues of $X(M)$, and their multiplicities, are determined by the weight enumerator of the code.

16.9 Linear Graphs are Hamming Quotients

There is a second useful description of linear graphs. We have constructed them as Cayley graphs $X(M)$, where M is a generator matrix of a code. If M is a generator matrix for a code C, then the kernel of M is the *dual code* $C^\perp$ of C. It is a code of the same length as C and, if C has length m, then $\dim(C^\perp) = m - \dim(C)$. Of course $(C^\perp)^\perp = C$. A code C is *self-orthogonal* if $C \le C^\perp$ and it is *self dual* if $C = C^\perp$.

Suppose $\mathbb{F}$ has order q and D is subspace of $\mathbb{F}^m$. The *coset graph* of D is the multigraph with the cosets of D as its vertices, and the number of edges joining two cosets equal to the number of elements in the second coset at Hamming distance one from an element of the second coset. Equivalently, the coset graph of D is the quotient of the Hamming graph $H(m, q)$ relative to the partition formed by the cosets of D.

If C is the dual code of D and M is a generator matrix for C, then $H(n, q)/D$ is isomorphic to the Cayley graph $X(M)$. (Exercise.)

Every linear Cayley graph is a coset graph relative to a code with minimum distance three. So we can take the vertices to be cosets of a subspace, and two cosets are adjacent if a word in one coset is at Hamming distance one from a word in the second. We can construct the eigenvectors from the characters of the additive group $\mathbb{F}^m$: if ψ is such a character, then the associated eigenvector of the quotient is the function $\hat{\psi}$ that maps a coset to the sum of the values of ψ on the coset.

16.10 Cubelike Graphs

The d-cube is an example of a Cayley graph for $\mathbb{Z}_2^d$. A Cayley graph $X(C)$ for $\mathbb{Z}_2^d$ has the binary vectors of length d as its vertices, with two vertices adjacent if and only if their difference lies in some specified subset C of $\mathbb{Z}_2^d \setminus \{0\}$. (The set C is the *connection set* of the Cayley graph.) If we choose C to consist of the d vectors from the standard basis of $\mathbb{Z}_2^d$, then the cubelike graph $X(C)$ is the d-cube. In [26] Facer, Twamley and Cresser showed that perfect state transfer occurs in a special class of Cayley graphs for $\mathbb{Z}_2^d$ that includes the d-cube, and this was extended to an even larger class of graphs in [10] by Bernasconi, Godsil and Severini.

If we let σ denote the sum of the elements of C, then the main result of [10] is that, if $\sigma \neq 0$, then at time $\pi/2$ we have perfect state transfer from u to $u + \sigma$, for each vertex u. Our goal is to study the situation when $\sigma = 0$; we find a surprising connection to binary codes.

If $u \in \mathbb{Z}_2^d$, then the map

$$x \mapsto x + u$$

is a permutation of the elements of $\mathbb{Z}_2^d$, and thus it can be represented by a $2^d \times 2^d$ permutation matrix P_u. We note that $P_0 = I$,

$$P_u P_v = P_{u+v}$$

and so $P_u^2 = I$. We also see that $\operatorname{tr}(P_u) = 0$ if $u \neq 0$ and

$$\sum_{u \in \mathbb{Z}_2^d} P_u = J.$$

16.10.1 Lemma. *If $C \subseteq \mathbb{Z}_2^d \backslash 0$ and X is the cubelike graph with connection set C, then $A(X) = \sum_{u \in C} P_u$.* □

If σ is the sum of the elements of C, then

$$P_\sigma = \prod_{u \in C} P_u.$$

16.10.2 Lemma. *If $U(t)$ is the transition operator of the cubelike graph $X(C)$, then $U(t) = \prod_{u \in C} \exp(itP_u)$.*

Proof. If matrices M and N commute then

$$\exp(M + N) = \exp(M)\exp(N)$$

Since $A = \sum_{u \in C} P_u$ and since the matrices P_u commute, the lemma follows. □

Suppose P is a matrix such that $P^2 = I$. Then

$$\exp(itP) = I + itP - \frac{t^2}{2!}I - i\frac{t^3}{3!}P + \frac{t^4}{4!}I + \cdots$$

and hence

$$\exp(itP) = \cos(t)I + i\sin(t)P.$$

If P is a permutation matrix we see that

$$\exp(\pi i P) = -I, \quad \exp\left(\frac{1}{2}\pi i P\right) = iP.$$

This implies that we have perfect state transfer on K_2 at time $\pi/2$, and that K_2 is periodic with period π.

If H is the transition operator for a Cayley graph of an abelian group then the argument used above shows that H can be factorized as a product of transition operators for a collection of perfect matchings and 2-regular subgraphs. Unfortunately this does not seem to allow us to derive useful information about state transfer.

Now we present a new and very simple proof of Theorem 1 from Bernasconi et al [10].

16.10.3 Theorem. *Let C be a subset of $\mathbb{Z}_2^d$ and let σ be the sum of the elements of C. If $\sigma \neq 0$, then perfect state transfer occurs in $X(C)$ from u to $u+\sigma$ at time $\pi/2$. If $\sigma = 0$, then X is periodic with period $\pi/2$.*

Proof. Let $U(t)$ be the transition operator associated with A. Then by 16.10.2
$$U(t) = \prod_{u \in C} \exp(itP_u).$$
From our remarks above
$$\exp(itP_u) = \cos(t)I + i\sin(t)P_u$$
and therefore
$$U(\pi/2) = \prod_{u \in C} iP_u = i^{|C|} P_\sigma.$$
This proves both claims. □

We show how to use these ideas to arrange for perfect state transfer from 0 to a specified vertex u in a cubelike graph. Assume we have cubelike graph with connection set C and let σ be the sum of the elements of C. If $\sigma = u$ then we already have transfer to u. First assume $\sigma = 0$. If $u \in C$ let C' denote $C \setminus u$; if $u \notin C$ let C' be $C \cup u$. In both cases the sum of the elements of C' is u and we're done. If $\sigma \neq 0$, replace C by $(C \setminus \sigma)$, now we are back in the first case. We can summarize this as follows. Let $S \oplus T$ denote the symmetric difference of the sets S and T.

16.10.4 Lemma. *If u is a vertex in the cubelike graph $X(C)$, then there is a connection set C' such that $|C \oplus C'| \leq 2$ and we have perfect state transfer from 0 to u in $X(C')$ at time $\pi/2$.* □

16.11 The Minimum Period

In this section we determine the minimum period of a cubelike graph.

We consider the spectral decomposition of the adjacency matrix of a cubelike graphs. If $a \in \mathbb{Z}_2^d$, then the function
$$x \mapsto (-1)^{a^T x}$$

is both a character of $\mathbb{Z}_2^d$ and an eigenvector of $X(C)$ with eigenvalue

$$\sum_{c \in C} (-1)^{a^T c}.$$

Let M be the matrix with the elements of C as its columns. Its row space is a binary code, and if $\mathrm{wt}(x)$ denotes the Hamming weight of x, the above eigenvalue is equal to

$$|C| - 2\,\mathrm{wt}(a^T M).$$

Thus the weight distribution of the code determines the eigenvalues of $X(C)$, and also their multiplicities. As a pertinent example we offer

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}$$

which has weight enumerator

$$x^{11} + 10x^7y^4 + 16x^5y^6 + 5x^3y^8,$$

from which we learn that the weights of its code words are 0, 4, 6 and 8. The eigenvalues of the associated cubelike graph are

$$11,\ 3,\ -1,\ -5$$

with respective multiplicities

$$1,\ 10,\ 16,\ 5.$$

If we define the $2^d \times 2^d$ matrix E_a by

$$(E_a)_{u,v} := 2^{-d}(-1)^{a^T(u+v)}$$

then $E_a^2 = E_a$ and, if $a \neq b$, then $E_a E_b = 0$. The columns of E_a are eigenvectors for $X(C)$ with eigenvalue $|C| - 2\,\mathrm{wt}(a^T M)$, and if $m = |C|$ we have

$$A = \sum_a (m - 2\,\mathrm{wt}(a^T M)) E_a.$$

More significantly

$$\begin{aligned}\exp(iAt) &= \sum_a \exp(i(m - 2\,\mathrm{wt}(a^T M))t)E_a \\ &= \exp(imt) \sum_a \exp(-2it\,\mathrm{wt}(a^T M))E_a\end{aligned}$$

With the eigenvalues in hand, our next result follows immediately from Theorem **??**.

16.11.1 Lemma. *Let X be a cubelike graph and let D be the greatest common divisor of the weights of the words in its code. Then the minimum period of X is π/D.* □

16.12 Characterizing State Transfer on Cubelike Graphs

We show how the existence of perfect state transfer on a cubelike graph can be read off from the associated binary code.

16.12.1 Theorem. *Let X be a cubelike graph with matrix M and suppose c is a vertex in X distinct from 0. Then the following are equivalent:*

(a) There is perfect state transfer from 0 to c.

(b) All words in C have weight divisible by D and $D^{-1}\,\mathrm{wt}(a^T M)$ and $a^T c$ have the same parity for all vectors a.

(c) D divides $|\mathrm{supp}(u) \cap \mathrm{supp}(v)|$ for any two code words u and v.

Further, if perfect state transfer occurs, it occurs at time $\pi/2D$.

Proof. We start by proving that (a) and (b) are equivalent. Perfect state transfer occurs at time $\pi/2D$ if and only if there is a complex scalar β of norm 1 and a permutation matrix T of order two and with trace zero such that

$$U(\pi/2D) = \beta T.$$

Now

$$(U(\pi/2D))_{0,c} = \exp(im\pi/2D) \sum_a \exp(-i\pi\,\mathrm{wt}(a^T M)/D)(E_a)_{0,c}$$

and

$$(E_a)_{0,c} = 2^{-d}(-1)^{a^Tc},$$

consequently

$$\begin{aligned}\beta\exp(-im\pi/D) &= 2^{-d}\sum_a \exp(-i\pi\,\mathrm{wt}(a^TM)/D)(-1)^{a^Tc}\\ &= 2^{-d}\sum_a (-1)^{\mathrm{wt}(a^TM)/D}(-1)^{a^Tc}.\end{aligned}$$

Here the left side of this equation has absolute value 1 and the right side is the average of 2^d numbers of absolute value 1, so the left side is ±1 and the summands on the right all have the same sign. So this equation holds if and only if, for all a we have

$$\frac{\mathrm{wt}(a^TM)}{D} = a^Tc, \quad (\text{modulo } 2).$$

Now this holds if and only if, modulo 2,

$$\frac{\mathrm{wt}((a+b)^TM)}{D} = \frac{\mathrm{wt}(a^TM)}{D} + \frac{\mathrm{wt}(b^TM)}{D}$$

for all a and b. This holds in turn if and only if, for any two code words u and v, we have that

$$\mathrm{wt}(u+v) = \mathrm{wt}(u) + \mathrm{wt}(v) \pmod{2D}$$

and this holds if and only if

$$|\operatorname{supp}(u)\cap\operatorname{supp}(v)| = 0 \pmod{D}. \qquad \square.$$

Suppose $\mathcal{C}$ is a binary code with generator matrix M. Let M' denote M viewed as a 01-matrix over $\mathbb{Z}$ and let Δ be the gcd of the entries in $M'\mathbf{1}$. Then the entries of $\Delta^{-1}M'\mathbf{1}$ are integers, not all even, and we define the image of this vector in $\mathbb{Z}_2$ to be the *center* of $\mathcal{C}$. Note that Δ is the gcd of the weights of the code words formed by the rows of M and, if Δ is odd, then the centre of $\mathcal{C}$ is equal to $M\mathbf{1}$.

16.12.2 Corollary. *Suppose X is a cubelike graph and c is a vertex in X distinct from 0. If we have perfect state transfer from 0 to c, then c is the centre of the code.* $\square$

Suppose x and y are binary vectors and Δ divides the weight of x, y and $x+y$. If

$$\mathrm{wt}(x) = a+b, \quad \mathrm{wt}(y) = a+c; \quad \mathrm{wt}(x+y) = b+c$$

then, modulo Δ,

$$\begin{aligned} a+b \qquad &= 0 \\ a \qquad + c &= 0 \\ b + c &= 0. \end{aligned}$$

This implies that, modulo Δ,

$$2a = 2b = 2c = 0.$$

It follows that the odd integer d divides the weight of each word in a binary code if and only if, for any two words x and y, the size of $\mathrm{supp}(x) \cap \mathrm{supp}(y)$ is divisible by d.

16.13 Examples

A code is *even* if D is even and *doubly even* if D is divisible by four. If C is even and the size of the intersection of any two code words is even, then C is self-orthogonal. Note that since our graphs are simple, their generator matrices cannot have repeated columns. (Using the standard terminology our codes are projective or, equivalently, the minimum distance of the dual is at least three.) So cubelike graphs with perfect state transfer at time $\pi/4$ correspond to self-orthogonal projective binary codes that are even but not doubly even.

Unpublished computations by Gordon Royle have provided a complete list of the cubelike graphs on 32 vertices. Analysis of the graphs in this list that show there are exactly six cubelike graphs on 32 vertices for which the codes are self-orthogonal and even but not doubly-even. The example in 16.11 is the one of these with least valency. These six graphs split into three pairs, each the complement of the other. In general, if perfect state transfer occurs on a graph it need not occur on its complement. In our case it must, as the following indicates. We use $\overline{X}$ to denote the complement of X.

16.13.1 Lemma. *If X is a cubelike graph with at least eight vertices then perfect state transfer occurs on X if and only if it occurs on $\overline{X}$.*

Proof. Since $A(\overline{X}) = J - I - A(X)$ we have.

$$U_{\overline{X}}(t) = \exp(it(J - I - A)).$$

If X is regular then J and A commute and

$$U_{\overline{X}}(t) = \exp(it(J - I))U_X(-t)$$

and hence

$$U_{\overline{X}}(\pi/k) = \exp(-i\pi/k)\exp((\pi i/k)J)U_X(\pi/k)^{-1}$$

If $|V(X)| = n$ then the eigenvalues of J are 0 and n and $\exp((\pi/k)J) = I$ provided n/k is even. □

There are a further six cubelike graphs on 32 vertices whose codes are doubly even. A doubly even code is necessarily self-orthogonal. If perfect state transfer occurs at time τ, then Lemma 5.2 in [19] yields that $\mathrm{tr}(U(\pi/4))$ must be zero, and using this we can show that perfect state transfer does not occur on these graphs. Thus we do not have examples of cubelike graphs with $D > 2$ where perfect state transfer occurs.

If M and N are binary matrices, their *direct sum* is the matrix

$$\begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix}$$

and the code of this matrix is the direct sum of the codes of M and N. If the code of M is self-orthogonal and even but not doubly even, then the direct sum of two copies of this code is all these things too. If X and Y are the cubelike graphs belonging to M and N, then the cubelike graph belonging to the direct sum of M and N is the Cartesian product of X and Y. The transition matrix of the Cartesian product of X and Y is $U_X \otimes U_Y$. One consequence is that we do have infinitely many examples of cubelike graphs admitting perfect state transfer at time $\pi/4$.

16.14 Cayley Graphs for $\mathbb{Z}_4^d$

We turn to Cayley graphs for $\mathbb{Z}_4^d$.

16.14.1 Lemma. *If $P^4 = I$, then*

$$\exp(itP) = \frac{1}{2}(I - P^2 + (P + P^{-1})(\cos(2t)P + \sin(2t)I))$$

and consequently

$$\exp\left(\frac{1}{2}\pi iP\right) = -P^2.$$

16.14.2 Lemma. *Suppose X is a Cayley graph for $\mathbb{Z}_4^d$ with connection set $\mathcal{C}$. Let $\mathcal{C}_1$ be the set of involutions in $\mathcal{C}$, and let $\mathcal{C}_2$ be the elements of order four. Let $P_1, \ldots, P_\ell$ be the permutation matrices corresponding to the elements of $\mathcal{C}_1$. Let $Q_1, \ldots, Q_m$ be the distinct permutation matrices corresponding to the squares of the elements in $\mathcal{C}_2$ (so $2m = |\mathcal{C}_2|$). Then*

$$U_X(\pi/2) = i^\ell \prod_{r=1}^{\ell} P_r \, (-1)^m \prod_{s=1}^{m} Q_s.$$

16.14.3 Corollary. *Let $X = X(\mathbb{Z}_4^d, \mathcal{C})$ and suppose all elements in $\mathcal{C}$ have order four. Let $\mathcal{D}$ be the set of squares of elements of $\mathcal{C}$. Then we have perfect state transfer on X at time $\pi/2$ if and only if we have perfect state transfer at time $\pi/2$ on the cubelike graph $X(\mathbb{Z}_2^d, \mathcal{D})$.* □

Notes

Exercises

Chapter 17

Uniform Mixing

We say that *instantaneous uniform mixing* occurs on X if there is a time τ such that

$$M_X(\tau) = \frac{1}{|V(X)|} J.$$

(Equivalently, $U(\tau)$ is flat.) We will abbreviate instantaneous uniform mixing to uniform mixing, as often as possible. As we have seen, for K_2 we have

$$U_{K_2}(\pi/4) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}$$

and therefore we have uniform mixing at time $\pi/4$. As we also saw in Section **??**, uniform mixing does not occur on K_n if $n > 4$. It is not hard to calculate that we have uniform mixing on K_3 at time $2\pi/9$, and on K_4 at time $\pi/4$. It follows that we have uniform mixing on the Hamming graphs $H(n,3)$ and $H(n,4)$ at the same times (respectively), since these graphs are Cartesian powers (of K_3 and K_4 respectively).

Since we have uniform mixing at $\pi/4$ for both K_2 and K_4, it follows that we also have uniform mixing on the Cartesian product $H(m,2) \,\square\, H(n,4)$ at $\pi/4$.

A flat unitary matrix is more often referred to as a *complex Hadamard matrix*. We say that a complex Hadamard matrix has *Butson index* m if its entries are m-th roots of unity. So a complex Hadamard matrix of Butson index two is just a Hadamard matrix. In design theory the term "complex Hadamard matrix" may sometimes be taken to mean "complex Hadamard matrix with Butson index four", i.e., with entries in $\{\pm 1, \pm i\}$.

If we do not have uniform mixing as just defined, it is possible that there is a vertex a such that the vector $e_a^T U(t)$ is flat. In this case we say that we have *local uniform mixing* at a.

17.1 Uniform Mixing on Cones

We first present examples of graphs which admit uniform mixing starting from a vertex. Carlson et al. [17] showed that there is uniform mixing on the star $K_{1,n}$, starting from the vertex of degree $n-1$. We prove a related result.

17.1.1 Lemma. *If Y is a regular with valency at most two and Z is the cone over Y, then Z admits local uniform mixing starting from the conical vertex.*

Proof. Assume $n = |V(Y)|$ and that Y is ℓ-regular. Denote the cone over Y by Z and let a denote the conical vertex. We set

$$\Delta = \sqrt{\ell^2 + 4n}$$

and recall from Section 12.1 that the eigenvalues in the eigenvalue support of a are

$$\frac{1}{2}(\ell \pm \Delta).$$

We denote these by μ_1 and μ_2, assuming that $\mu_1 > \mu_2$.

If $y \in V(Y)$ then Lemma 12.3.1 yields that

$$U_Z(t)_{a,y} = \frac{1}{\Delta}\left(\mathrm{e}^{\mathrm{i}t\mu_1} - \mathrm{e}^{\mathrm{i}t\mu_2}\right) = \frac{\mathrm{e}^{\mathrm{i}t\mu_2}}{\Delta}\left(\mathrm{e}^{\mathrm{i}t\Delta} - 1\right).$$

We note that this is independent of the choice of y in Y, and conclude that we have uniform mixing from a if and only if there is a time t such that

$$\frac{1}{\Delta}|\mathrm{e}^{\mathrm{i}t\Delta} - 1| = \frac{1}{\sqrt{n+1}};$$

equivalently we need

$$|\mathrm{e}^{\mathrm{i}t\Delta} - 1| = \frac{\sqrt{\ell^2 + 4n}}{\sqrt{n+1}}.$$

As $\ell^2 + 4n = \ell^2 - 4 + 4n + 4$, the ratio on the right lies in the interval $[0, 2]$ if and only if $\ell \leq 2$. Hence in these cases we can find a time t which satisfies this equation, and then we have uniform mixing starting from a. □

By taking Cartesian powers, we get further examples with uniform mixing starting from one vertex of the graph, as

$$\exp(\mathrm{i}t(Z\Box Z))e_{(a,a)} = \exp(\mathrm{i}tZ)e_a \otimes \exp(\mathrm{i}tZ)e_a.$$

It seems plausible that, in most cones, we do not get uniform mixing starting from a the vertex in the base graph, but we do not have a proof in general. We leave it as an exercise to show that we do not get uniform mixing in $K_{1,n}$ starting from a vertex of degree one. You might also show that if X has at least two vertices and Y at least three, then in the join $X+Y$ we cannot have uniform mixing starting from a vertex in X.

Hanmeng Zhan has observed that we do have uniform mixing on $K_{1,3}$ at time $2\pi/3\sqrt{3}$, and hence on its Cartesian powers at the same time. These are our only examples of graphs that admit uniform mixing and are not regular.

17.2 Transcendental Numbers

We have already met some basic number theory when we introduced algebraic numbers and explored some of their properties in Chapter 7. It turns out however that most numbers are not roots of polynomials with integer coefficients, and these are called transcendental numbers. Proving that a number is transcendental is typically no trivial task. From the late 19th century to the early 20th, a sequence of now famous results established the foundations of what is known as transcendental number theory. They culminated in theorem proved independently by A. Gel'fond and Th. Schneider in 1934, which solved Hilbert's seventh problem.

17.2.1 Theorem (Gelfond-Schneider)**.** *If α and β are algebraic numbers, with $\alpha \neq 0, 1$ and $\beta \notin \mathbb{Q}$, then α^β is transcendental.*

An equivalent form, which will be more useful to us, states that if $\alpha \neq 0$ and $\beta \notin \mathbb{Q}$ are complex numbers, then at least one of the numbers e^α, β and $\mathrm{e}^{\alpha\beta}$ is transcendental. This will be used to show that some restrictions on the eigenvalues of matrices where uniform mixing occurs.

For this next result, recall from Chapter 7 that the set of algebraic numbers form an algebraically closed field.

17.2.2 Theorem. *Let X be a graph, $A = A(X)$. Assume that for a given $t \neq 0$, there is a matrix M, with all of its entries algebraic numbers, so that $U(t) = \lambda M$, with $\lambda \in \mathbb{C}$. Then the ratio of any two non-zero eigenvalues of X is a rational number.*

Proof. Assume $A = \sum_{r=0}^{d} \theta_r E_r$ is the spectral decomposition of A. First,

$$\det \exp(\mathrm{i}tA) = \prod_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} = \mathrm{e}^{\mathrm{i}t\,\mathrm{tr}(A)} = 1.$$

Thus $\lambda^n \det M = 1$, and therefore, as the entries of M are algebraic, we have that λ must be algebraic. Thus all entries of $U(t)$ are algebraic numbers, whence the roots of its characteristic polynomial are also algebraic numbers, that is, $\{\mathrm{e}^{\mathrm{i}t\theta_0}, ..., \mathrm{e}^{\mathrm{i}t\theta_d}\}$ are algebraic numbers.

Take any two distinct θ_r and θ_s, with $\theta_s \neq 0$, and assume θ_r/θ_s is not rational. From the Gelfond-Schneider Theorem, one of the numbers

$$\frac{\mathrm{i}t\theta_r}{\mathrm{i}t\theta_s}, \quad \mathrm{e}^{\mathrm{i}t\theta_s}, \quad \mathrm{e}^{\mathrm{i}t\theta_s(\theta_r/\theta_s)}$$

is transcendental. The first cannot be because θ_r and θ_s are algebraic, and the second and third cannot be from our previous discussion. Thus θ_r/θ_s must be rational. □

When we are guaranteed that the ratio of any two non-zero eigenvalues is a rational number, it is enough to find one non-zero integral eigenvalue to conclude that all other eigenvalues must also be integers. Regular graphs provide a large class of examples of graphs with at least one integral eigenvalue.

17.2.3 Corollary. *If X is a regular graph, and if, for a given $t \neq 0$, there is a matrix M, with all of its entries algebraic numbers, so that $U(t) = \lambda M$ for some $\lambda \in \mathbb{C}$, then all eigenvalues of X are integers.* □

In view of the result above, it seems natural to pursue a classification of uniform mixing in regular graphs, and, naturally, dealing with few eigenvalues is preferable. As we have already discussed, the complete graphs K_2, K_3 and K_4 admit uniform mixing, but no other complete graph does. In the next sections, we intend to classify the strongly regular graphs that admit uniform mixing.

17.3 Regular Hadamard Matrices

We introduce a largish class of graphs that admit uniform mixing. To begin with, we vary our setup, and use symmetric Hadamard matrices (rather than adjacency matrices) as Hamiltonians. Suppose H is a symmetric $n \times n$ Hadamard matrix. Then $H^2 = nI$ and if $\hat{H} := n^{-1/2}H$, we find that

$$\begin{aligned}\exp(\mathrm{i}t\hat{H}) &= I + \mathrm{i}t\hat{H} - \frac{t^2}{2} - \mathrm{i}\frac{t^3}{6}\hat{H} + \cdots \\ &= \cos(t)I + \mathrm{i}\sin(t)\hat{H}.\end{aligned}$$

So $\exp(\frac{1}{2}\pi\mathrm{i}\hat{H}) = \mathrm{i}\hat{H}$ and we have uniform mixing at time $\pi/2$; if we use H in place of $\hat{H}$ we have uniform mixing at time $\pi/(2\sqrt{n})$.

The matrix

$$A = \frac{1}{2}(H + J)$$

is a 01-matrix and we can analyse the continuous quantum walk on it if H and J commute, that is, if H is a regular symmetric Hadamard matrix. If H is regular and symmetric with row sum k, we have

$$n\mathbf{1} = H^2\mathbf{1} = H(k\mathbf{1}) = k^2\mathbf{1}$$

and therefore the order n must be a perfect square. Now

$$\exp(\mathrm{i}tA) = \exp\left(\frac{\mathrm{i}t}{2}(H + J)\right) = \exp\left(\frac{\mathrm{i}t}{2}J\right)\exp\left(\frac{\mathrm{i}t}{2}H\right).$$

We have

$$\exp(\mathrm{i}(t/2)J) = \frac{\mathrm{e}^{\mathrm{i}(t/2)n}}{n}J + I - \frac{1}{n}J = I - \frac{1}{n}(1 - \mathrm{e}^{\mathrm{i}(t/2)n})J$$

which is equal to I when $(t/2)n$ is an even multiple of π. Thus, if $t = \pi/(2\sqrt{n})$, we have that $\exp(\mathrm{i}tA)$ is flat when

$$\frac{n}{4\sqrt{n}} = 2m$$

for some integer m, and hence we conclude that uniform mixing takes place on A if $n = 64m^2$, that is, if n is a perfect square and 64 divides n.

If A has 0 diagonal, then it is the adjacency matrix of a regular graph. Further, $A^2 = (1/4)(nI + 2kJ + nJ)$, and therefore A is the adjacency matrix of a strongly regular graph with parameters

$$(n,\ (n+k)/2;\ (n+2k)/4,\ (n+2k)/4).$$

17.4 Conference Graphs

A *conference graph* on q vertices is a strongly regular graph with parameters

$$q,\ \frac{q-1}{2};\ \frac{q-5}{4},\ \frac{q-1}{4}.$$

For an immediate example we have C_5. The complement of a conference graph is again a conference graph (and so conference graphs are cospectral to their complements). The eigenvalues of a conference graph on q vertices are its valency $(q-1)/2$ (with multiplicity one) and

$$\frac{1}{2}(-1 \pm \sqrt{q}),$$

both with multiplicity $(q-1)/2$ (thus immediately implying that q must be odd). Conference graphs can be characterized by the fact that the multiplicities of their non-trivial eigenvalues are equal. One can further restrict the possible number of vertices in a conference graph with the following result, which we state without a proof.

17.4.1 Lemma. *If X is a conference graph of order n, then n is congruent to 1 modulo 4, and n is the sum of two squares.* □

The matrix of eigenvalues P for the association scheme of a conference graph on q vertices is

$$\begin{pmatrix} 1 & \frac{q-1}{2} & \frac{q-1}{2} \\ 1 & \frac{-1+\sqrt{q}}{2} & \frac{-1-\sqrt{q}}{2} \\ 1 & \frac{-1-\sqrt{q}}{2} & \frac{-1+\sqrt{q}}{2} \end{pmatrix},$$

from which we can confirm that this scheme is formally self-dual.

The best known examples of conference graphs are the *Paley graphs*, constructed as follows. Let $\mathbb{F}$ be a finite field of order q, where $q \equiv 1$ modulo 4. The elements of $\mathbb{F}$ are the vertices of the Paley graph, and two vertices are adjacent if their difference is a non-zero square in $\mathbb{F}$. The Paley graphs are self-complementary. The eigenvalues of a Paley graph are integers if and only if q is a square. The Paley graph on 9 vertices is isomorphic to $K_3 \,\square\, K_3$ and therefore admits uniform mixing at time $2\pi/9$. However Mullin [**?**] proved that this is the only conference graph where uniform mixing occurs.

Recall that if X is strongly regular, then its adjacency algebra is spanned by I, A and $\overline{A} = A(\overline{X})$. Any matrix which is a polynomial in A is a linear combination of the three matrices above, thus, if uniform mixing occurs, there is a flat unitary W so that $W = \alpha I + \beta A + \gamma \overline{A}$. Following Mullin, we determine the flat unitary matrices in the adjacency algebra of a conference graph. Recall, from Theorem 14.11.1, that a flat unitary is a scalar multiple of a type-II matrix.

17.4.2 Lemma. *Let X be a conference graph on q vertices with adjacency matrix A. If W is a flat type-II matrix in the adjacency algebra of X with diagonal entries equal to 1, then*

$$W = I + xA + x^{-1}\overline{A}$$

where $|x| = 1$ and

$$x + x^{-1} = \frac{-2 \pm 2\sqrt{q}}{q-1}.$$

Proof. Let $c = (q-1)/4$. Thus, the parameters of X are $(4c+1,\ 2c;\ c-1,\ c)$. If

$$W = I + xA + y\overline{A}$$

then

$$\begin{aligned} WW^{(-T)} &= (I + xA + y\overline{A})(I + x^{-1}A + y^{-1}\overline{A}) \\ &= I + A^2 + \overline{A}^2 + (x + x^{-1})A + (y + y^{-1})\overline{A} + (xy^{-1} + x^{-1}y)A\overline{A} \end{aligned}$$

If we expand A^2, $\overline{A}^2$ and $A\overline{A}$ in terms of I, A and $\overline{A}$, knowing that $A^2 = (2c)I + (c-1)A + c\overline{A}$, we find that

$$WW^{(-T)} = nI + w_1 A + w_2 \overline{A}$$

where

$$\begin{aligned} w_1 &= 2c - 1 + c(xy^{-1} + x^{-1}y) + x + x^{-1}, \\ w_2 &= 2c - 1 + c(xy^{-1} + x^{-1}y) + y + y^{-1}. \end{aligned}$$

If W is to be a type-II matrix, then $w_1 = w_2 = 0$. If $w_1 = w_2$, then

$$x + x^{-1} = y + y^{-1}$$

and since $|x| = |y| = 1$ because W is flat, it follows that $x = y$ or $x = y^{-1}$.

If $x = y$, the first equation of the pair of equations becomes

$$0 = 4c - 1 + x + x^{-1},$$

and since $|x + x^{-1}| \leq 2$, this has no solution when $n \geq 5$.

Hence $x = y^{-1}$ and our two equations reduce to the single equation

$$0 = 2c - 1 + c(x^2 + x^{-2}) + x + x^{-1}.$$

If we set $\sigma = x + x^{-1}$, we can rewrite this as a quadratic

$$0 = c\sigma^2 + \sigma - 1,$$

from which it follows that

$$\sigma = \frac{-2 \pm 2\sqrt{n}}{n-1}. \qquad \square$$

Our goal in the next section is to show the all but one conference graph admits uniform mixing. With that mind, we first derive an important consequence of duality. Since the association scheme of a conference graph is formally self-dual, Theorems 14.11.1 and 9.7.2 give the following immediately.

17.4.3 Lemma. *Let X be a conference graph and let E_0, E_1, E_2 be its spectral projections. Then $I + xA + y\overline{A}$ is a flat type-II matrix if and only if $E_0 + xE_1 + yE_2$ is flat and unitary.* $\square$

17.5 Uniform Mixing on Strongly Regular Graphs

In this section we prove that the Paley graph on nine vertices is the only conference graph that admits uniform mixing. This result appears in [?], but we are following the treatment in Mullin [?].

17.5.1 Theorem. *The only conference graph that admits uniform mixing is the Paley graph on nine vertices.*

Proof. Let X be a conference graph on n vertices, with adjacency matrix A and spectral projections E_0, E_1 and E_2. Assume uniform mixing occurs in X at time t.

If n is not a square, the non-trivial eigenvalues of X are irrational. On the other hand, $U(t)$ is flat and unitary, thus a multiple of a type-II matrix by Theorem 14.11.1. Lemma 17.4.2 says that this type-II matrix is algebraic, therefore, as a consequence Corollary 17.2.3, the eigenvalues of X would have to be integers.

So $n = m^2$ for some m, and n is odd. If $m = 3$, it is well known that X must be the Payley graph of order 9. We see below that this is the only case indeed.

Having $U(t) = \sum_{r=0}^{2} \mathrm{e}^{\mathrm{i}t\theta_r} E_r$ flat and unitary, Lemma 17.4.3 implies that

$$M = I + \mathrm{e}^{\mathrm{i}t(\theta_1-\theta_0)} E_1 + \mathrm{e}^{\mathrm{i}t(\theta_2-\theta_0)} E_2$$

is a flat type-II matrix. From Lemma 17.4.2, two consequences unfold: $\mathrm{e}^{\mathrm{i}t(\theta_1-\theta_0)} = \mathrm{e}^{-\mathrm{i}t(\theta_2-\theta_0)}$, and thus $\mathrm{e}^{-n\mathrm{i}t} = 1$; and

$$2\cos(t(\theta_1-\theta_0)) = \mathrm{e}^{\mathrm{i}t(\theta_1-\theta_0)} + \mathrm{e}^{-\mathrm{i}t(\theta_1-\theta_0)} = \frac{-2 \pm 2\sqrt{n}}{n-1}.$$

17.6 Cycles

We show that uniform mixing does not take place on even cycles, or on cycles of prime length.

17.6.1 Lemma. *If we have uniform mixing on a bipartite graph X, then the ratios of the eigenvalues of X are rational. If X is also regular, its eigenvalues are integers.*

Proof. Assume $n = |V(X)|$. As we saw in Section 1.8, if the transition matrix $U(t)$ of a bipartite graph is flat, then the entries of $\sqrt{n}$ are ± 1 or $\pm i$; hence they are algebraic. Now apply Lemma **??**.

If X is regular then its valency is an integer eigenvalue, and therefore all eigenvalues are integers. □

17.6.2 Theorem. *The only cycle of even length that admits uniform mixing is C_4.*

Proof. [*** to go here ***]

For cycles of odd length we work harder to say less:

17.6.3 Theorem. *If p is prime and $p > 3$, then uniform mixing does not occur on C_p.*

Proof. Haagerup has proved that there are only finitely many type-II matrices in the Bose-Mesner algebra of a cycle of prime order. By Corollary 14.12.2 it follows that the entries of any such type-II matrix are algebraic. By Theorem **??** we see that if uniform mixing occurs then the eigenvalues of the cycle must be integers. Therefore we cannot have uniform mixing on C_p, for any prime greater than three. □

17.7 A Flat Unitary Circulant

We say that *ϵ-uniform mixing* occurs on the graphs X if, for each positive real ϵ there is a time t such that

$$\|U(t) \circ U(t)^* - n^{-1}J\| < \epsilon.$$

You may show that if X admits uniform mixing, so do its Cartesian powers.

We aim to show that each cycle of prime length admits ϵ-uniform mixing, but for this some non-trivial preparation is required. The material in this section is a lightly edited version of material from [**?**, Section 9].

We rely on the viewpoint of cyclic association schemes. Let p denote an odd prime and consider the cycle C_p. Let $d = \lfloor \frac{p}{2} \rfloor$. For $0 \le r \le d$ we define the following adjacency matrices.

$$[A_r]_{j,k} = \begin{cases} 1, & \text{if } j-k \in \{r, -r\} \pmod p; \\ 0, & \text{otherwise.} \end{cases}$$

Note that A_0 is the $p \times p$ identity matrix, and A_1 is the adjacency matrix of the cycle C_p. Let $\mathcal{A} = \{A_0, \ldots, A_d\}$. The set of matrices $\mathcal{A} = \{A_0, \ldots, A_d\}$ form the *cyclic association scheme* of order p.

It is also convenient to consider the underlying permutation matrix C that is the adjacency matrix of a directed cycle. We index the rows and columns of C with elements of $\mathbb{Z}_p$ such that

$$C_{j,k} = \begin{cases} 1, & \text{if } j-k \equiv 1 \pmod p \\ 0, & \text{otherwise.} \end{cases}$$

Let $\mathcal{A} = \{A_0, \dots, A_d\}$ denote the cyclic association scheme on p vertices. Since p is an odd prime, we see that $\mathcal{A}$ has $d = (p-1)/2$ classes. We further let $\{E_0, \dots, E_d\}$ denote the spectral idempotents of $\mathcal{A}$. We assume that these idempotents have been ordered such that $E_0 = \frac{1}{p}J$ and

$$E_r = \sum_{j=0}^{n-1} \left(\omega^{jr} + \omega^{-jr}\right) C^j.$$

for $1 \le r < \lfloor n/2 \rfloor$.

We define

$$F = \sum_{r=0}^{d} \omega^{r^2} E_r, \tag{17.7.1}$$

where $\omega = e^{i2\pi/p}$.

17.7.1 Lemma. *The matrix F is a flat unitary matrix.* □

Proof. First we verify that F is unitary. We do this by a direct computation. It is convenient to recall that

$$E_r^2 = E_r \quad \text{and} \quad E_r E_j = 0 \ \text{ if } \ r \neq j.$$

Using these observations we see that

$$FF^* = \left(\sum_{r=0}^{d} \omega^{r^2} E_r\right)\left(\sum_{r=0}^{d} \omega^{-r^2} E_r\right) = \sum_{r=0}^{d} E_r = I.$$

Next we use the discrete Fourier transform Θ to show that F is flat. Note that for an arbitrary matrix M in $\mathbb{C}[\mathcal{A}]$ there exists a unique polynomial $p(x)$ of degree at most $p-1$ in $\mathbb{C}[x]$ such that $M = p(C)$. Further note that Θ is defined such that

$$\Theta(M) = \sum_{j=0}^{n-1} p(\omega^j) C^j.$$

Since Θ is linear, we have

$$\begin{aligned}\Theta(F)\Theta(F^*) &= \left(\sum_{r=0}^{d} \omega^{r^2}\Theta(E_r)\right)\left(\sum_{r=0}^{d} \omega^{-r^2}\Theta(E_r)\right)\\ &= \left(\sum_{r=0}^{d} \omega^{r^2}A_r\right)\left(\sum_{r=0}^{d} \omega^{-r^2}A_r\right)\\ &= \left(\sum_{j=0}^{p-1} \omega^{j^2}C^j\right)\left(\sum_{j=0}^{p-1} \omega^{-j^2}C^j\right)\\ &= \sum_{k=0}^{p-1}\left(\sum_{j=0}^{p-1} w^{j^2-(k-j)^2}\right)C^k\\ &= \sum_{k=0}^{p-1}\omega^{-k^2}\left(\sum_{j=0}^{p-1} w^{jk}\right)C^k\\ &= pC^0\\ &= pI.\end{aligned}$$

By a well-known property of the discrete Fourier transform, we know that $\Theta(F)\Theta(F^*) = pI$ implies that

$$F \circ F^* = \frac{1}{p}J.$$

Therefore F is flat. □

17.8 ϵ-Uniform Mixing on C_p

Our goal now is to show that $U(t)$ gets arbitrarily close to a complex scalar multiple of F as t ranges over all real numbers. Since F is a flat matrix, achieving this goal implies that C_p admits ϵ-uniform mixing. The proof of this result relies heavily on Kronecker's Theorem. Again it is a lightly edited version of the argument presented in [**?**, Section 9].

17.8.1 Theorem. *For each odd prime p, the cycle C_p admits ϵ-uniform mixing.*

Proof. Let $U'(t)$ denote the scaled transition matrix given by

$$U'(t) = e^{-2it}U(t) = E_0 + e^{(\theta_1-2)it}E_1 + \cdots + e^{(\theta_d-2)it}E_d. \tag{17.8.1}$$

Note that $U'(t)$ is a unitary matrix, and $U'(t)$ is flat if and only if $U(t)$ is flat. Let ϵ denote a positive real number. We proceed by showing that there exists some time t such that

$$\|U'(t) - F\| < \frac{\epsilon}{2}.$$

We consider $U'(t)$ at times that are an integer multiple of $2\pi/p$. For any s in $\mathbb{Z}$, we see that Equation 17.8.1 becomes

$$U'(2s\pi/p) = \sum_{r=0}^{d} e^{2s(\theta_r - 2)\pi i/p} E_r.$$

In terms of e, we express Equation 17.7.1 as

$$F = \sum_{r=0}^{d} e^{2r^2\pi i/p} E_r.$$

Our goal is to find a time t such that the coordinates of F and $U'(t)$ are close to the same value. In terms of the exponents of these coefficients, this is equivalent to finding some integer s such that $\frac{1}{p}r^2 \approx \frac{1}{p}(\theta_r - 2)s$ in $(\mathbb{R}/\mathbb{Z})$ for $0 \le r \le d$. For two elements x and y in $\mathbb{R}/\mathbb{Z}$, we define the distance $|x-y|_{\mathbb{R}/\mathbb{Z}}$ to be

$$|x-y|_{\mathbb{R}/\mathbb{Z}} = \inf_{k\in\mathbb{Z}}\{|x-y-k|\},$$

where the norm on the right hand side of the definition is the absolute value of $x - y - k$ considered as a real number.

From Theorem **??**, we know that

$$\{1, \theta_1, \ldots, \theta_{d-1}\}$$

is linearly independent over $\mathbb{Q}$, and consequently

$$\left\{1, \frac{1}{p}(\theta_1 - 2), \ldots, \frac{1}{p}(\theta_{d-1} - 2)\right\}$$

is linearly independent over the rationals.

By Kronecker's Theorem (Theorem **??**), we see that

$$D = \left\{\left(\frac{1}{p}(\theta_1 - 2)s, \ldots, \frac{1}{p}(\theta_{d-1} - 2)s\right) : s \in \mathbb{Z}\right\}$$

is dense in $(\mathbb{R}/\mathbb{Z})^{d-1}$.

Therefore for any $\delta > 0$, we can find some s in $\mathbb{Z}$ such that

$$\left|\frac{1}{p}(\theta_r - 2)s - \frac{r^2}{p}\right|_{\mathbb{R}/\mathbb{Z}} < \delta \tag{17.8.2}$$

in $(\mathbb{R}/\mathbb{Z})$ for all $1 \leq r \leq d-1$. It remains to consider the coordinates of $U'(t)$ and F with respect to E_d. Recall that for a cyclic association scheme we have

$$\theta_d = -1 - \theta_1 - \theta_2 \cdots - \theta_{d-1}.$$

We can use this to derive an expression for the d-th coordinate of $U'(t)$ in terms of the first $d-1$ coordinates.

$$\begin{aligned}\frac{1}{p}(\theta_d - 2)s &= \frac{1}{p}\left(-3 - \sum_{r=1}^{d-1}\theta_r\right)s \\ &= -\frac{1}{p}(2(d-1)+3)s - \sum_{r=1}^{d-1}\frac{1}{p}(\theta_r - 2)s \\ &= -s - \sum_{r=1}^{d-1}\frac{1}{p}(\theta_r - 2)s.\end{aligned}$$

Now working in $\mathbb{R}/\mathbb{Z}$, we see that the exponent of the d-th coordinate of $U'(t) - F$ is

$$\frac{1}{p}(\theta_d - 2)s - \frac{1}{p}d^2 = -s - \sum_{r=1}^{d-1}\frac{1}{p}(\theta_r - 2)s - \frac{1}{p}d^2 \tag{17.8.3}$$

$$= \sum_{r=1}^{d-1}\left(\frac{1}{p}(\theta_r - 2)s - \frac{1}{p}r^2\right) + \frac{1}{p}\sum_{r=0}^{d} r^2. \tag{17.8.4}$$

Note that

$$\frac{1}{p}\sum_{r=1}^{d} r^2 = \frac{d(d+1)(2d+1)}{6p} = \frac{(p-1)(p+1)}{24}$$

Since p is an odd prime, we know that both $p-1$ and $p+1$ are even, and exactly one of those values is divisible by 4. Therefore $(p-1)(p+1)$ is divisible by 8. Since we are assuming that $p \neq 3$, we also know that $p-1$ or $p+1$ is divisible by 3. It follows that

$$\frac{(p-1)(p+1)}{24} \in \mathbb{Z}.$$

must be an integer. We simplify Equation 17.8.3 in $\mathbb{R}/\mathbb{Z}$ to

$$\frac{1}{p}(\theta_d - 2)s - \frac{1}{p}d^2 = \sum_{r=1}^{d-1} \left(\frac{1}{p}(\theta_r - 2)s - \frac{1}{p}r^2 \right).$$

Now we use this expression and Inequality 17.8.2 to bound the coefficient d-th coordinate of $U'(t) - F$ in terms of δ as follows:

$$\left| \frac{1}{p}(\theta_d - 2)s - \frac{1}{p}d^2 \right|_{\mathbb{R}/\mathbb{Z}} \leq \sum_{r=1}^{d-1} \left| \frac{1}{p}(\theta_r - 2)s - \frac{1}{p}r^2 \right|_{\mathbb{R}/\mathbb{Z}} < (d-1)\delta.$$

This implies that for any $\epsilon > 0$, we can find a sufficiently small δ such that

$$\|U'(2s\pi/p) - F\| < \frac{\epsilon}{2}.$$

It can be shown that if A and B are symmetric $n \times n$ complex matrices, such that

$$\|A - B\| \leq \gamma,$$

for some positive real number γ. Then

$$\|A \circ A^* - B \circ B^*\| \leq 2\gamma.$$

Therefore it follows that

$$\|U'(2s\pi/p) \circ U'(2s\pi/p)^* - \frac{1}{n}J\| < \epsilon.$$

Finally, we note that

$$U'(2s\pi/p) \circ U'(2s\pi/p)^* = U(2s\pi/p) \circ U(2s\pi/p)^*,$$

which proves that ϵ-uniform mixing occurs on C_p. □

17.9 Cubelike Graphs

The graphs K_2 and K_4 are the first two members of a series of graphs: folded cubes. The *folded* $(d+1)$*-cube* is the graph we get from the d-cube by joining each vertex to the unique vertex at distance d from itself. It can also be viewed as the quotient of the $(d+1)$-cube over the equitable partition formed by the pairs of vertices at distance $d+1$, which is the origin of the term 'folding'. The first interesting example is the folded 5-cube, often known as the Clebsch graph. In [11] Best et al. prove (in our terms) that when d is odd, the folded d-cube has uniform mixing. The Hamming graph $H(n,q)$ has instantaneous uniform mixing if and only if $q \le 4$. (Exercise: show that if a Cartesian power of X has uniform mixing, then so does X.)

We view cubelike graphs as quotients of the d-cube. The latter admits uniform mixing at $\pi/4$; we want to determine the quotients that admit uniform mixing at the same time. Let A the adjacency matrix for Q_d. There is an equitable partition σ with normalized characteristic matrix S, such that $AS = SB$ where B is the adjacency matrix of the quotient. Since the cells of σ are cosets of a subgroup Γ, they all have the same size; since we assume our subgroup has minimum distance at least three, the quotient Q_d/σ is a simple graph. So

$$U_A(t)S = SU_B(t)$$

and therefore

$$U_B(t) = S^T U_A(t) S.$$

If $|\Gamma| = 2^e$, it follows that each entry of $U_B(t)$ is the row sum of a block in the block partition of $U_A(t)$ determined by σ.

Let $\mathrm{wt}(x)$ denote the Hamming weight of x. For the d-cube

$$(U(\pi/4))_{a,b} = i^{\mathrm{wt}(a-b)}$$

Hence we are dealing with sums

$$R_c := \sum_{x\in\Gamma} i^{\mathrm{wt}(c-x)}$$

for $c \in \mathbb{Z}_2^d$, and so our problem "reduces" to questions about the weight distribution of cosets of Γ.

An example. Suppose Γ is the subgroup of order two generated by $\mathbf{1} = \Big(1,1,\dots,1\Big)$. If $\mathrm{wt}(c) = w$, then $\mathrm{wt}(c-\mathbf{1}) = d-w$ and

$$R_c = i^w + i^{d-w} = i^r(1+i^{d-2w}) = i^r(1+(-1)^w i^d).$$

If d is odd, $R_c = i^d(1\pm i)$. Hence $|R_c|$ is independent of c and we have proved that we have uniform mixing on the folded d-cube when d is odd.

(We note that K_4 is the first example, since it is the folded 3-cube.) This example was first found by Tamon et. al [**?**].

If d is even, say $d = 2e$, then $R_c = i^w(1 + (-1)^{w+e})$. In this case $|R_c|$ is 0 or $2i^r$, depending on the parity of $w = \text{wt}(c)$. This we get uniform distribution on words whose weight has the same parity as e.

A second example. Suppose $d = 2e$ and x and y are words of weight e such that $x+y = \mathbf{1}$. Take Γ to be $\{0, x, y, \mathbf{1}\}$. If $\text{wt}(c) = w$ and $\text{wt}(x \circ c) = v$ then $\text{wt}(y \circ c) = w - v$. Hence

$$\text{wt}(c - x) = e + w - 2v, \quad \text{wt}(c - y) = e - (w - 2v)$$

and accordingly

$$\begin{aligned} R_c &= i^w + i^{e+w-2v} + i^{e-w+2v} + i^{2e-w} \\ &= i^w + (-1)^v(i^{e+w} + i^{e-w}) + (-1)^{e+w} i^w \\ &= i^w(1 + (-1)^{e+w}) + (-1)^v i^{e+w}(1 + (-1)^w) \end{aligned}$$

If e is odd, then either $1 + (-1)^{e+w} = 0$ or $1 + (-1)^w = 0$, but not both. So if e is odd then $|R_c| = 2$ and we have uniform mixing. But this graph is just the Cartesian square of the folded e-cube.

If we apply the first construction with $d = 5$, our quotient is the folded 5-cube, which is 5-regular on 16 vertices. Applying the second with $d = 6$ yields a 6-regular graph on 16 vertices.

On four vertices, the cubelike graphs with uniform mixing are C_4 and K_4, and on eight vertices we have the 3-cube Q_3 and $K_2 \,\square\, K_4$. On 16 we see Q_4, $C_4 \,\square\, K_4$ and $K_4 \,\square\, K_4$ (with valencies respectively 4, 5 and 6). Since $C_4 \,\square\, K_4$ has girth three and the folded 5-cube girth five, these graphs are not isomorphic.

The following result is [**?**,].

17.9.1 Lemma. *If $\Gamma = \langle a, b \rangle$ is a subgroup of $\mathbb{Z}_2^d$, then the quotient $H(d, 2)/\Gamma$ admits uniform mixing at time $\pi/4$ if either*

(a) $\text{wt}(a) \equiv \text{wt}(b)$ *(mod 4) and* $\text{wt}(a + b) \equiv 2$ *(mod 4), or*

(b) $\text{wt}(a) \equiv \text{wt}(b) + 2$ *(mod 4) and* $\text{wt}(a + b) \equiv 0$ *(mod 4).*

We are not restricted to time $\pi/4$, as the following result of Chan shows.

17.9.2 Lemma. *The distance-r graph of $H(2^d - 8, 2)$ admits uniform mixing at time $\pi/2^{d-2}$.*

(Here the connection set consists of all words of weight r.)

17.10 Other Groups

We know less about groups other than $\mathbb{Z}_2^d$. Natalie Mullin proved that if $d \equiv 0, 2 \pmod 3$ then the "folding" $H(d,3)/\langle \mathbf{1} \rangle$ admits uniform mixing at time $2\pi/9$. Harmony Zhan proved the following.

17.10.1 Lemma. *If $\Gamma = \langle a, b \rangle$ is a sugroup of $\mathbb{Z}_3^d$, then the quotient graph $H(d,2)/\Gamma$ admits uniform mixing at time $2\pi/9$ if either*

(a) $a^T b \equiv 0$ (mod 3), $\mathrm{wt}(a) \not\equiv 0$ and $\mathrm{wt}(b) \equiv 0$ (mod 3), or

(b) $a^T b \not\equiv 0$ (mod 3), and $\mathrm{wt}(a) \not\equiv \mathrm{wt}(b)$ unless $\mathrm{wt}(a) \equiv \mathrm{wt}(b) \equiv 0$ (mod 3).

Zhan also proved that the distance-r graph of $H(2 \cdot 3^k - 9, 3)$ admits uniform mixing at time $2\pi/3^k$ if

$$r \in \{3^k - 1, 3^k - 4, 3^k - 7\}.$$

For $\mathbb{Z}_4^d$, Mullin show that when d is even, the folding $H(d,4)/\langle \mathbf{1} \rangle$ admits uniform mixing at time $\pi/4$. Zhan showed that the distance-2^{d-1} graph of $H(2^{d-1}, 4)$ admits uniform mixing at time $\pi/2^{d+1}$, as do the distance-$(2^{d-1} - 1 - 1)$ and distance 2^{d-1} of $H(2^d - 2, 4)$.

Aside from the following, due to Zhan, we have very little information about when uniform mixing can occur. (Here ϕ is the Euler totient function.)

17.10.2 Theorem. *If $X(\mathbb{Z}_2^d, \mathcal{C})$ admits uniform mixing at time π/n, then $|\mathcal{C}| \geq \phi(n) + 1$. If $X(\mathbb{Z}_3^d, \mathcal{C})$ admits uniform mixing at time π/n, then $|\mathcal{C}| \geq \phi(n) + 2$.*

Mullin has conjectured that uniform mixing does not occur on $\mathbb{Z}_p^d$ if $p \geq 5$.

Notes

Exercises

Part V

Back Matter

Chapter 18

Problems with Quantum Walks

We list some open problems.

18.1 State Transfer

18.1.1 Question. *Are there graphs on which perfect state transfer occurs between vertices a and b, and the sum of the eigenvalues in the eigenvalue support of a is not zero?*

18.1.2 Question. *Is there a tree with more than three vertices on which perfect state transfer occurs?*

This question may be too difficult, so we pose a related question.

18.1.3 Question. *Is there a positive integer D such that no tree of diameter greater than D admits perfect state transfer?*

18.1.4 Question. *Is it true that, for a positive real c, there are only finitely many connected graphs with average valency at most c on which perfect state transfer takes place?*

Of course a tree has average valency less than two.

Our next question has very little to do with state transfer, but we find it interesting.

18.1.5 Question. *If there a tree with three pairwise strongly cospectral vertices?*

18.1.6 Question. *Let $D(X,a)$ be the graph we get by taking two (vertex-disjoint) copies of the graph X rooted at v, and adding an edge joining the two copies of a. If X is a tree, can we have perfect state transfer between the two copies of a in $D(X,a)$.*

We know that the copies of a in $D(X,a)$ are strongly cospectral. The question is also of interest when X is not a tree.

18.1.7 Question. *Let Y be the graph obtained from the graph X by adding two new vertices, each adjacent to the same vertex a of X. Find examples of graphs Y, with at least four vertices, such that we have perfect state transfer between the two new vertices.*

The two new vertices are strongly cospectral if the multiplicity of 0 as an eigenvalue of $X \setminus a$ is not greater than its multiplicity on X. (If $X = K_1$, this condition holds and Y is $K_{1,2}$, which does admit perfect state transfer between its end-vertices.)

We consider a sequence of rooted graphs (X,a). The continuous quantum walks on the graphs are *sedentary* at the vertex a if there is a constant c such that

$$|U_X(t)_{a,a}| \geq 1 - \frac{c}{|V(X)|}.$$

for all but finitely many graphs in the sequence. A sequence of graphs is *sedentary* if the above bound holds for all X and for all vertices a of X. Amazingly, the complete graphs are sedentary! Many families of strongly regular graphs are also sedentary.

18.1.8 Question. *Is there a sedentary family of connected cubic graphs?*

18.2 Pretty Good State Transfer

18.2.1 Question. *For which graphs X do the graphs $D(X,a)$ admit pretty good state transfer between the root vertices?*

Examples where X is a star are known. The question is interesting even for trees and, although we ask for a characterization, even just a good number of examples would be significant.

18.2.2 Question. *Let Y be the graph obtained from the graph X by adding two new vertices, each adjacent to the same vertex a of X. Are there graphs Y, with at least four vertices, such that we have pretty good state transfer between the two new vertices?*

One difficulty with pretty good state transfer is that to get high fidelity, it is necessary to wait a long time. However Chen, Mereau and Feder [?] have shown that by weighting edges, this difficulty can be avoided. Their example is obtained from the path P_n (where $n \geq 6$) by joining new vertices to 3 and $n-2$ by an edge of weight w. Pretty good state transfer takes place between vertices 1 and n.

18.2.3 Question. *Find more examples where we can get rapid, high fidelity, pretty good state transfer by weighting one or two edges.*

18.3 Real State Transfer

Suppose $S \subseteq V(X)$ and let D be the diagonal 01-matrix with $D_{i,i} = 1$ if and only if $i \in S$. Then we say S is *periodic* if there is a non-zero time t such that

$$U(t)DU(-t) = D.$$

Replacing S by its complement $\overline{S}$ and D by $I - D$, we see that S is periodic if and only if $\overline{S}$ is. Since D is a projection, S is periodic if and only if $\operatorname{col}(D)$ is a $U(t)$-invariant subspace of $\mathbb{C}^{V(X)}$.

18.3.1 Question. *Find examples of periodic subsets S such that $|S| \geq 3$ and the subgraph induced by S is a clique or coclique.*

Practically all work on continuous quantum walks concerns the situation where the initial state is of the $e_a e_a^T$, and if work is concerned with state transfer, then the final state is also of this form. If a and b are vertices of X, we define

$$D_{a,b} = (e_a - e_b)(e_a - e_b)^2.$$

We describe states of this form as *pair states* and if $a \sim b$, as *edge states*. If $a \sim b$ then $D_{a,b}$ is the Laplacian of the edge $\{a, b\}$, and the Laplacian of X is a sum of such edge-Laplacians. Chen has investigated perfect state transfer between edge states in her M.Math. thesis [?]. She has shown that we have perfect edge state transfer on the path P_n if and only if $n = 2, 3$.

18.3.2 Question. *Is there perfect edge-state transfer on some tree with more than three vertices?*

Note that it is possible to have perfect state transfer from an edge state to a non-edge state but, other than the fact that it is possible, we know very little.

18.4 Walks on Oriented Graphs

An *oriented graph* X is a directed graph where any two distinct vertices are joined by at most one arc. It is convenient to represent an oriented graph by a skew-symmetric matrix S where $S_{i,j}$ is 1 if ij is an arc in X, -1 if ji is an arc, and is zero otherwise. If S is skew-symmetric, then $\exp(S)$ is an orthognal matrix. Hence

$$U(t) := \exp(tS)$$

determines a quantum walk. (If S is skew symmetric, $U(t) = \exp(-it(iS))$ and iS is Hermitian, thus our Hamiltonian is hermitian as usual.) Bipartite graphs provide an interesting class of examples: if X is bipartite with adjacency matrix

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

then

$$\begin{pmatrix} iI & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} -iI & 0 \\ 0 & I \end{pmatrix} = \begin{pmatrix} 0 & iB \\ -iB^T & 0 \end{pmatrix}.$$

Hence the matrices

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}, \quad i \begin{pmatrix} 0 & B \\ -B^T & 0 \end{pmatrix}$$

are unitarily similar, and so information about quantum walks on oriented graphs can provide information about quantum walks on bipartite graphs.

We say that *multiple state transfer* takes place on an oriented graph X if there is perfect state-transfer between each pair of vertices in S. Cameron et al noted that if X is K_3, then multiple state transfer takes place on $S = V(X)$. Lato [?] provides an example of a graph on 8 vertices where multiple state transfer occurs on a subset of four vertices.

18.4.1 Question. *Find more examples of multiple state transfer.*

Preferably an infinite family.

18.5 Uniform Mixing

The only even cycle that admits uniform mixing is C_4. Mullin has shown that no cycle of prime length admits uniform mixing.

18.5.1 Question. *Which odd cycles admit uniform mixing?*

The first open case for this question is C_9. The only graphs we know that are not regular and admit uniform mixing are the Cartesian powers of $K_{1,3}$.

18.5.2 Question. *Find graphs that are not regular, are not Cartesian powers of $K_{1,3}$, and which admit uniform mixing.*

18.5.3 Question. *Which trees admit local uniform mixing relative to some vertex?*

The following two conjectures are due to Mullin.

18.5.4 Conjecture. *If a graph admits uniform mixing at time t, then e^{it} is a root of unity.*

18.5.5 Conjecture. *If $n \geq 5$, no connected Cayley graph for $\mathbb{Z}_n^d$ admits uniform mixing.*

18.6 Average Mixing

It has been shown that if the average mixing matrix of a graph on n vertices is $\frac{1}{n}J$, then $n \leq 2$. It is not hard to show that a doubly stochastic matrix with rank one is equal to $\frac{1}{n}J$. So there are only two connected graphs with average mixing matrix of rank one.

18.6.1 Question. *Are there infinitely many graphs with average mixing matrix of rank two?*

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