1 Introduction

These lectures entitled:

Quantum Probability and Applications to Complex Networks

are intended to present a quantum probabilistic approach to spectral analysis of complex networks. For a technical reason these lectures are divided into two parts:

Part 1 (March–April) Quantum Probabilistic Aspect of Adjacency Algebras

Keywords: adjacenct matrix, characteristic polynomial, spectrum, adjacency algebra, distance-regular graph, quantum decomposition, interacting Fock space, orthogonal polynomial, continued fraction, Cauchy-Stieltjes transform, etc.

Part 2 (May-June) Spectral Analysis of Large Complex Networks

Keywords: tree, Wigner semicircle law, growing graph, quantum central limit theorem, asymptotic spectrum, random graph, Watts–Strogatz model, etc.

1.1 Complex Networks

In the real world one finds networks in their basic form as interrelations among objects. Such networks are described in terms of graph theory, namely, objects under consderation being set as points in a plane and two objects in interrelation being connected by an arc therein, we obtain a geometric description of the network called a graph (in fact, the mathematical definition of a graph makes us to abandon even such a geometric image).

The graph theory, tracing back to Euler's famous problem on seven bridges in Königsberg, has become one of the main subjects in discrete mathematics. From mathematical point of view most attention has been paid to "beautiful" graphs, e.g., reasonable size for handling and/or possessing nice symmetry, but little to very large graphs in the real world because of being "dirty" or "complex." Examples of such dirty graphs are telephone networks, the internet (physical connections among PC's), the WWW (hyperlinks of webpages), Hollywood costars, coauthors of articles, human or social relations, biological networks, etc.

During the last decade as the development of computer technology, some characteristics became computable for very large networks in the real world. As a few physical quantities are used efficiently for description of gas in stead of the set of huge number of Newton equations, we believe reasonably that such large networks can be captured in terms of a small number of statistical characteristics carefully chosen. Up to now the prevailing characteristics of large complex networks in the real worlds are:

- 1. Small world phenomenon dating back to Stanley Milgram's small world experiment (1967), saying that the mean distance of two vertices is small $O(\log n)$ relative to the large number n of vertices.
- 2. Large cluster coefficient ($C \ge 0.7$), i.e., locally most vertices are connected each other.
- 3. Existence of hubs, as indicated by the long tail of the power law degree distribution $p(k) \propto k^{-\gamma} \ (\gamma > 1).$



Figure 1.1: The internet

Mathematical models for complex networks were proposed in the following epoch-making papers:

- D. J. Watts and S. H. Strogatz: Collective dynamics of 'small-world' networks, Nature 393 (1998), 440–442.
- [2] A.-L. Barabási and R. Albert: Emergence of scaling in random networks, Science 286 (1999), 509–512.

Since then up to now many papers have been published with only few mathematical rigorous results. Our intention is to develop mathematical study of those models as well as to propose new models. For a mathematical model of a large complex network, a single graph seems to be not suitable. In order to capture characteristics of their large size we reasobnably take a growing graph and study its asymptotic behavior. And for characteristics of its complexity it is natural to consider statistical quantities of a random ensemble of graphs. In these lectures, therefore, one should keep in mind that a graph is intended to grow and/or to be random.

1.2 Quantum Probability = Noncommutative Probability

Quantum probability theory provides a framework of extending the measure-theoretical (Kolmogorovian) probability theory. The idea traces back to von Neumann (1932), who, aiming at the mathematical foundation for the statistical questions in quantum mechanics, initiated a parallel theory by making a selfadjoint operator and a trace play the roles of a random variable and a probability measure, respectively.

One of the main purposes of these lectures is to test the quantum probabilistic techniques in the study of large complex networks, in particular, their spectral properties.



Figure 1.2: Paul Erdös' coauthors

1.3 From Coin-toss to Graph Spectrum

1.3.1 Classical probabilistic model

The toss of a fair coin is modelled by a random variable X on a probability space (Ω, \mathcal{F}, P) satisfying the property:

$$P(X = +1) = P(X = -1) = \frac{1}{2}$$

Rather than the random variable itself more essential is the probability distribution of X defined by

$$\mu = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_{+1} \tag{1.1}$$

The moment sequence is one of the most fundamental characteristics of a probability measure. For μ in (1.1) the moment sequence is calculated with no difficulty as

$$M_m(\mu) = \int_{-\infty}^{+\infty} x^m \mu(dx) = \begin{cases} 1, & \text{if } m \text{ is even,} \\ 0, & \text{otherwise.} \end{cases}$$
(1.2)

When we wish to recover a probability measure from the moment sequence, we meet in general a delicate problem called *determinate moment problem*. For the coin-toss there is no such an obstacle and we can recover the Bernoulli distribution from the moment sequence.



Figure 1.3: High school dating

1.3.2 Quantum probabilistic (matrix) model

We set

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad e_0 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$
(1.3)

Then $\{e_0, e_1\}$ is an orthonormal basis of the two-dimensional Hilbert space \mathbb{C}^2 and A is a selfadjoint operator acting on it. It is straightforward to see that

$$\langle e_0, A^m e_0 \rangle = \begin{cases} 1, & \text{if } m \text{ is even,} \\ 0, & \text{otherwise,} \end{cases}$$
(1.4)

which coincides with (1.2). In other words, the coin-toss is modeled also by using the two-dimensional Hilbert space \mathbb{C}^2 and the matrix A. In our terminology, letting \mathcal{A} be the *-algebra generated by A, the coin-toss is modeled by an algebraic random variable A in an algebraic probability space (\mathcal{A}, e_0) . We call A an *algebraic realization* of the random variable X.

1.3.3 Noncommutative Structure

Once we come to an algebraic realization of a classical random variable, we are naturally led to the non-commutative paradigm. Let us consider the decomposition

$$A = A^{+} + A^{-} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix},$$
 (1.5)

which yields a simple proof of (1.4). In fact, note first that

$$\langle e_0, A^m e_0 \rangle = \langle e_0, (A^+ + A^-)^m e_0 \rangle = \sum_{\epsilon_1, \dots, \epsilon_m \in \{\pm\}} \langle e_0, A^{\epsilon_m} \cdots A^{\epsilon_1} e_0 \rangle.$$
(1.6)

Let \mathcal{G} be a connected graph consisting of two vertices e_0, e_1 . Observing the obvious fact that (1.6) coincides with the number of *m*-step walks starting at and terminating at e_0 (see the figure below), we obtain (1.4).



Thus, computation of the *m*th moment of A is reduced to counting the number of certain walks in a graph through (1.5). This decomposition is in some sense canonical and is called the *quantum decomposition* of A.

1.3.4 Relation to Graph

We now note that A in (1.3) is the adjacency matrix of the graph \mathcal{G} . Having established the identity

$$\langle e_0, A^m e_0 \rangle = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots,$$
 (1.7)

we say that μ is the spectral distribution of A in the state e_0 . In other words, we obtain an integral expression for the number of returning walks in the graph by means of such a spectral distribution. A key role in deriving (1.7) is again played by the quantum decomposition.

1.4 Quantum Probabilistic Approach

For (in particular, asymptotic) spectral analysis some techniques peculiar to quantum probability seem to be useful. They are

- (a) quantum decomposition (using noncommutative structure behind)
- (b) various concepts of independence and corresponding quantum central limit theorems
- (c) partition statistics for computing the moments of spectral distributions

A basic reference throughout these lectures is:

[3] A. Hora and N. Obata: Quantum Probability and Spectral Analysis of Graphs, Springer, 2007.

2 Graphs and Adjacency Matrices

2.1 Graphs

Definition 2.1.1 Let V be a non-empty set and E a subset of $\{\{x, y\}; x, y \in V, x \neq y\}$. Then the pair G = (V, E) is called a *graph* with vertes set V and the edge set E. An element of V is called a *vertex* and an element of E an *edge*. We say that two vertices $x, y \in V$ are adjacent, denoted by $x \sim y$, if $\{x, y\} \in E$.

A geometric representation of a graph G = (V, E) is a figure obtained by assigning each $x \in V$ to a point in a plane and drawing a line (or an arc) between two planer points if they are adjacent in G. Appearance of the geometric representation of a graph varies widely. For example, the following two figures represent the same graph.

Figure 2.1: Two geometric representation of the Petersen graph

Definition 2.1.2 A graph G = (V, E) is called *finite* if V is a finite set, i.e., $|V| < \infty$.

Definition 2.1.3 For a vertex $x \in V$ of a graph G we set

$$\deg(x) = \deg_G(x) = |\{y \in V; y \sim x\}|,$$

which is called the *degree* of x.

Definition 2.1.4 A graph G = (V, E) is called *localy finite* if $deg(x) < \infty$ for all $x \in V$.

Definition 2.1.5 A graph G = (V, E) is called *regular* if every vertex has a constant finite degree, i.e., if there exists a constant number κ such that $\deg(x) = \kappa$ for all $x \in V$. To be more precise, such a graph is called κ -regular.

Definition 2.1.6 A finite sequence of vertices $x_0, x_1, \ldots, x_n \in V$ is called a *walk* of length n if

$$x_0 \sim x_1 \sim \dots \sim x_n \,, \tag{2.1}$$

where some of x_0, x_1, \ldots, x_n may coincide. A walk (2.1) is called a *path* of length n if x_0, x_1, \ldots, x_n are distinct from each other. A walk (2.1) is called a *cicle* of length $n \ge 3$ if $x_0, x_1, \ldots, x_{n-1}$ are distinct from each other and $x_n = x_0$.



2.2. ADJACENCY MATRICES

In usual we do not consider an orientation of a path. Namely, if (2.1) is a path,

$$x_n \sim x_{n-1} \sim \cdots \sim x_0$$

is the same path. For a cycle, we do not consider the initial vertex either. Namely, if $x_0 \sim x_1 \sim \cdots \sim x_{n-1} \sim x_0$ is a cycle, then $x_1 \sim x_2 \sim \cdots \sim x_{n-1} \sim x_0 \sim x_1$ stands for the same cycle.



Figure 2.2: P_5 : path of length 4 (left). C_5 : cycle of length 5 (right)

Definition 2.1.7 A graph G = (V, E) is *connected* if every pair of distinct vertices $x, y \in V$ $(x \neq y)$ are connected by a walk (or equivalently by a path).

Definition 2.1.8 Two graphs G = (V, E) and G' = (V', E') are called *isomorphic* if there exists a bijection $f : V \to V'$ satisfying

$$x \sim y \quad \Longleftrightarrow \quad f(x) \sim f(y).$$

In that case we write $G \cong G'$.

2.2 Adjacency Matrices

2.2.1 Definition

Let V and V' be arbitrary non-empty set. A function $a : V \times V' \to \mathbf{R}$ is regarded as a matrix A indexed by $V \times V'$ in the sense that the matrix element of A is defined by $(A)_{xy} = a(x, y)$. In this case we write $A = (a_{xy})$ too.

Definition 2.2.1 Let G = (V, E) be a graph. A matrix $A = (a_{xy})$ indexed by $V \times V$ is called the *adjacency matrix* of G if

$$a_{xy} = \begin{cases} 1, & \text{if } x \sim y, \\ 0, & \text{otherwise} \end{cases}$$

Lemma 2.2.2 Let V be a non-empty set. A matrix A indexed by $V \times V$ is the adjacency matrix of a graph G with V being the vertex set if and only if

- (i) $(A)_{xy} \in \{0, 1\};$
- (ii) $(A)_{xy} = (A)_{yx};$
- (iii) $(A)_{xx} = 0.$

PROOF. Obvious.

A matrix S indexed by $V \times V'$ is called a *permutation matrix* if

- (i) $(S)_{xy'} \in \{0, 1\};$
- (ii) $\sum_{y' \in V'} (S)_{xy'} = 1$ for all $x \in V$;
- (iii) $\sum_{x \in V} (S)_{xy'} = 1$ for all $y' \in V'$.

If S is a permutation matrix, it is necessary that |V| = |V'|.

The transposed matrix S^T is defined in a usual manner: $(S^T)_{y'x} = S_{xy'}$ for $x \in V$ and $y' \in V'$. Then $S^T = S^{-1}$ in the sense that SS^T is the identity matrix indexed by $V \times V$ and S^TS is the identity matrix indexed by $V' \times V'$.

Lemma 2.2.3 Let A and A' be the adjacency matrices of graphs G = (V, E) and G' = (V', E'), respectively. Then $G \cong G'$ if and only if there exists a permutation matrix S indexed by $V \times V'$ such that $A' = S^{-1}AS$

PROOF. Suppose that $G \cong G'$. We choose an isomorphism $f: V \to V'$ and define a matrix S indexed by $V \times V'$ by

$$(S)_{xy'} = \begin{cases} 1, & \text{if } y' = f(x), \\ 0, & \text{otherwise.} \end{cases}$$

We see easily that S is a permutation matrix satisfying SA' = AS.

Conversely, suppose that a permutation matrix S indexed by $V \times V'$ verifies $A' = S^{-1}AS$. Then a bijection $f: V \to V'$ is defined by the condition that

$$(A)_{xy} = \begin{cases} 1, & \text{if } y = f(x), \\ 0, & \text{otherwise.} \end{cases}$$

It is then easy to see that f becomes an isomorphism between G and G'.

2.2.2 Representing the Adjacency Matrix in a Usual Form

In order to represent the adjacency matrix A of a graph G = (V, E) in a usual form of $n \times n$ square matrix, where n = |V|, we need numbering the vertices. This is performed by taking a bijection $f: V \to \{1, 2, \ldots, n\} = V'$. Then we obtain a graph G' = (V', E') in such a way that $\{i, j\} \in E'$ if and only if $\{f^{-1}(i), f^{-1}(j)\} \in E$. By definition we have $G \cong G'$. The adjacency matrix A' of G' is indexed by $V' \times V'$ and admits a usual expression of a square matrix. It follows from Lemma 2.2.3 that A and A' are related as $A = SA'S^{-1}$.

Consider another numbering, that is, another bijection $f_1 : V \to \{1, 2, ..., n\} = V'$. Then we obtain another square matrix A'_1 as the adjacency matrix of G'_1 , which is related to A as $A = S_1 A'_1 S_1^{-1}$. Then we have

$$S_1 A_1' S_1^{-1} = S A' S^{-1}$$

so that

$$A_1' = S_1 S A' (S_1 S)^{-1}.$$

Note that S_1S is a usual permutation matrix on $\{1, 2, \ldots, n\}$. Consequently,

Lemma 2.2.4 Let A, A' be the adjacency matrices of a graph G obtained from two ways of numbering the vertices. Then there exists a permutation matrix on $\{1, 2, ..., n\}$, n = |V|, such that $A' = S^{-1}AS$.

Example 2.2.5 We obtain "different" adjacency matrices by different numbering the vertices of the same graph.



2.2.3 Some Properties in Terms of Adjacency Matrices

All the information of a graph (up to isomorphism) are obtained from its adjacency matrix.

(1) A graph G = (V, E) is not connected if and only if there exists a numbering the vertices such that the adjacency matrix admits a block diagonal expression of the form:

$$A = \begin{bmatrix} A_1 & O \\ O & A_2 \end{bmatrix} \qquad (A_1, A_2 \text{ are square matrices})$$

In this case A_1 and A_2 are the adjacency matrices of subgraphs of G which are not connected.

(2) A graph is called *complete* if every pair of vertices are connected by an edge. A comlete graph with n vertices is denoted by K_n . A graph is complete if and only if the adjacency matrix is of the form:

$$A = \begin{bmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 1 & \cdots & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & \cdots & & 0 & 1 \\ 1 & \cdots & & 1 & 0 \end{bmatrix}$$

(3) A graph G = (V, E) is called *bipartite* if V admits a partition $V = V_1 \cup V_2$, $V_1 \cap V_2 = \emptyset$, $V_1 \neq \emptyset$, $V_2 \neq \emptyset$, such that any pair of vertices in a common V_i does not constitute an edge. A graph is bipartite if and only if the adjacency matrix admits a block diagonal expression of the form:

$$A = \begin{bmatrix} O & B \\ B^T & O \end{bmatrix}$$
 (two zero matrices are square matrices).

(4) A graph G = (V, E) is called *complete bipartite* if it is bipartite and every pair of vertices $x \in V_1$, $y \in V_2$ constitute an edge. In that case we write $G = K_{m,n}$ with $m = |V_1|$ and $n = |V_2|$. In particular, $K_{1,n}$ is called a *star*.

A graph is complete bipartite if and only if the adjacency matrix is of the form:



Figure 2.3: Bipartite graph, complete bipartite graph $K_{4,5}$, star $K_{1,6}$

2.2.4 Generalization of Graphs

(1) Directed graph. One may consider naturally the case where every edge of a graph is given a direction. Such an object is called a *directed graph*. In terms of the adjacency matrix A, a directed graph is characterized by the following properties:

(i)
$$(A)_{xy} \in \{0, 1\};$$

(ii) $(A)_{xy} = 1$ implies $(A)_{yx} = 0;$

(iii)
$$(A)_{xx} = 0$$

(2) Multigraph. In its geometric representation one may allow to draw two or more edges connecting two vertices (multi-edge) and one or more arcs connecting a vertex with itself (loop). In terms of the adjacency matrix A, a directed graph is characterized by the following properties:

(i)
$$(A)_{xy} \in \{0, 1, 2, \dots\};$$

(ii)
$$(A)_{xy} = (A)_{yx}$$
.

Moreover, each edge may be given a direction to obtain a directed multigraph.

(3) Network. An arbitrary matrix gives rise to a graph where each directed edge \overrightarrow{xy} is associated with the value A_{xy} . Such an object is called generally a *network*. A transition diagram of a Markov chain is an example.

In regard to (1) and (2), a graph in these lectures is sometimes called a *undirected simple graph*.



Figure 2.4: Directed graph, multigraph, directed multigraph.

2.3 Characteristic Polynomials

Let G = (V, E) be a finite graph with |V| = n. Numbering the vertices, we write down its adjacency matrix in the usual form of an $n \times n$ matrix, say A. The characteristic polynomial of A is defined by

$$\varphi_A(x) = |xE - A| (= \det(xE - A)).$$

It is noted that $\varphi_A(x)$ is determined independently of the numbering. In fact, let A' be the adjacenct matrix obtained by a different numbering. From Lemma 2.2.4 we know that $A' = S^{-1}AS$ with a permutation matrix S. Then,

$$\varphi_{A'}(x) = |xE - A'| = |xE - S^{-1}AS| = |S^{-1}(xE - A)S| = |S^{-1}||xE - A||S| = \varphi_A(x).$$

We call $\varphi_A(x)$ the *characteristic polynomial* of G and denote it by $\varphi_G(x)$. Obviously, $\varphi_G(x)$ is a polynomial of degree n of the form:

$$\varphi_G(x) = x^n + c_1 x^{n-1} + c_2 x^{n-2} + c_3 x^{n-3} + \cdots .$$
(2.2)

Example 2.3.1 Simple examples are:



Example 2.3.2 One more example. The characteristic polynomial of the following graph is $\varphi(x) = x^4 - 4x^2 - 2x + 1$.



Theorem 2.3.3 Let the characteristic polynomial of a finite graph G be given as in (2.2). Then,

(1) $c_1 = 0.$

(2) $-c_2 = |E|.$ (3) $-c_3 = 2\Delta$, where Δ is the number of triangles in G.

PROOF. Let $A = [a_{ij}]$ be the adjacency matrix of G written down in the usual form of $n \times n$ matrix after numbering the vertices. Noting that the diagonal elements of A vanish, we see that the characteristic polynomial of G is given by

$$\varphi_G(x) = |xE - A| = \begin{vmatrix} x & -a_{12} & \cdots & -a_{1n} \\ -a_{21} & x & \cdots & -a_{2n} \\ \vdots & & \ddots & \vdots \\ -a_{n1} & \cdots & \cdots & x \end{vmatrix}.$$

For simplicity, the matrix in the right-hand side is denoted by $B = [b_{ij}]$. We then have

$$\varphi_G(x) = |B| = \sum_{\sigma \in \mathcal{S}(n)} \operatorname{sgn}(\sigma) b_{1\sigma(1)} b_{2\sigma(2)} \cdots b_{n\sigma(n)}.$$
(2.3)

For $\sigma \in \mathcal{S}_n$ we set

$$\operatorname{supp} \sigma = \{i \,|\, \sigma(i) \neq i\}.$$

Then (2.3) becomes

$$\varphi_G(x) = \sum_{k=0}^n \sum_{\substack{\sigma \in \mathcal{S}(n) \\ |\text{supp }\sigma| = k}} \operatorname{sgn}(\sigma) b_{1\sigma(1)} b_{2\sigma(2)} \cdots b_{n\sigma(n)} \equiv \sum_{k=0}^n f_n(x)$$
(2.4)

Since the indeterminat x appears only in the diagonal of B, we see that $f_n(x) = c_k x^{n-k}$.

(1) k = 1. Since there is no permutation σ such that $|\operatorname{supp} \sigma| = 1$, we have $c_1 = 0$.

(2) k = 2. The permutations σ satisfying $|\operatorname{supp} \sigma| = 2$ are parametrized as $\sigma = (i \ j)$ $(1 \le i < j \le n)$. For such a permutation we have $\operatorname{sgn}(\sigma) = -1$. Hence we have

$$f_2(x) = \sum_{1 \le i < j \le n} (-1)(-a_{ij})(-a_{ji})x^{n-2} = -\sum_{1 \le i < j \le n} a_{ij}x^{n-2}$$

where we used $a_{ij}a_{ji} = a_{ij}^2 = a_{ij}$. Therefore, $c_2 = -|E|$.

(3) k = 3. The permutations σ satisfying $|\operatorname{supp} \sigma| = 3$ are parametrized as

$$\sigma = (i \ j \ k), \quad \sigma = (i \ k \ j), \quad 1 \le i < j < k \le n.$$

Noting that sgn $(\sigma) = 1$ for such cyclic permutations, we have

$$f_3(x) = -\sum_{1 \le i < j < k \le n} (a_{ij}a_{jk}a_{ki} + a_{ik}a_{kj}a_{ji})x^{n-3}.$$

We see that $a_{ij}a_{jk}a_{ki}$ takes values 1 or 0 according as three vertices i, j, k forms a triangle or not. The same situation occuring for the second term, we conclude that $-c_3 = 2\Delta$.



Figure 2.5: Path P_n

2.4 The Path Graph P_n and Chebyshev Polynomials

Let $V = \{1, 2, ..., n\}$ and $E = \{\{i, i+1\}; i = 1, 2, ..., n-1\}$. The graph (V, E) is called a *path* with n vertices and is denoted by P_n .

Lemma 2.4.1 Let $\varphi_n(x) = \varphi_{P_n}(x)$ be the characteristic polynomial of the path P_n . The it holds that

$$\varphi_1(x) = x,$$

$$\varphi_2(x) = x^2 - 1,$$

$$\varphi_n(x) = x\varphi_{n-1}(x) - \varphi_{n-2}(x), \quad n \ge 3$$
(2.5)

PROOF. We have already seen in Example 2.3.1 that

$$\varphi_1(x) = x, \quad \varphi_2(x) = x^2 - 1.$$

Let us compute $\varphi_n(x)$ for $n \ge 3$. By definition we have

$$\varphi_n(x) = \begin{vmatrix} x & -1 \\ -1 & x & -1 \\ & -1 & x & -1 \\ & \ddots & \ddots & \ddots \\ & & -1 & x & -1 \\ & & & & -1 & x \end{vmatrix}$$

By cofactor expansion with respect to the first column, we get

$$\varphi_n(x) = \lambda \varphi_{n-1}(x) + \begin{vmatrix} -1 & -1 & & \\ x & -1 & & \\ -1 & x & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & x & -1 \\ & & & -1 & x \\ & & & -1 & x \end{vmatrix}$$
$$= x \varphi_{n-1}(x) - \varphi_{n-2}(x),$$

as desired.

Setting $\varphi_0(x) = 1$, we may understand that the reccurence relation in (2.5) holds for $n \ge 2$.

Lemma 2.4.2 For n = 0, 1, 2, ... there exists a polynomial $U_n(x)$ such that

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}.$$
 (2.6)

Moreover, $U_n(x)$ satisfies the following recurrence relation:

$$U_0(x) = 1, \quad U_1(x) = 2x, \quad U_{n+1}(x) - 2xU_n(x) + U_{n-1}(x) = 0.$$
 (2.7)

PROOF. By elementary knowledge of trigonometric functions.

Definition 2.4.3 The series of polynomials $U_n(x)$ is called the *Chebyshev polynomial of the second kind*.

Theorem 2.4.4 The characteristic polynomial of the path P_n is given by $U_n(x/2)$.

PROOF. Let $\varphi_n(x)$ be the characteristic polynomial of P_n . We see easily from (2.5) and (2.7) that the recurrence relations of $\varphi_n(x)$ and $U_n(x/2)$ coincide together with the initial conditions.

2.5 Exercises

(1) Let G = (V, E) be a graph with a vertex a of degree one. Let $b \in V$ be a unique vertex adjacent to a. Let $G' = G[V \setminus \{a\}], G'' = G[V \setminus \{a, b\}]$ be induced subgraphs obtained by deleting $\{a\}$ and $\{a, b\}$, respectively. Prove that

$$\varphi_G(x) = x\varphi_{G'}(x) - \varphi_{G''}(x).$$

(2) Compute the characteristic polynomial of the complete graph K_n . Then verify Theorem 2.3.3 directly.

Ans.
$$\varphi(x) = (x - (n - 1))(x + 1)^{n-1}$$
.

References

- [4] N. Biggs: Algebraic Graph Theory (2nd Edition), Cambridge University Press, Cambridge, 1993.
- [5] B. Bollobás: Modern Graph Theory, Graduate Texts in Mathematics Vol. 184, Springer-Verlag, New York, 1998.

3 Spectra of Graphs

3.1 Spectra

Let G = (V, E) be a finite graph with |V| = n and let A be the adjacency matrix represented in a usual form of $n \times n$ matrix after numbering the vertices. Since A becomes a real symmetric matrix, its eigenvalues are all real, say, $\lambda_1 < \lambda_2 < \cdots < \lambda_s$. Then, the characteristic polynomial of G is factorized as

$$\varphi_G(x) = (x - \lambda_1)^{m_1} \cdots (x - \lambda_s)^{m_s}, \qquad (3.1)$$

where $m_i \ge 1$ (called the multiplicity of λ_i) and $\sum_i m_i = n$.

Definition 3.1.1 Let G = (V, E) be a finite graph and let $\varphi_G(x)$ its characteristic polynomial in the form (3.1). The the array

$$\operatorname{Spec}\left(G\right) = \left(\begin{array}{ccc}\lambda_{1} & \lambda_{2} & \cdots & \lambda_{s}\\ m_{1} & m_{2} & \cdots & m_{s}\end{array}\right)$$
(3.2)

is called the spectrum of G. Each λ_i is called an eigenvalue of G and m_i its multiplicity.

In fact, (3.2) is nothing else the spectrum of the adjacency matrix A. Obviously, (3.2) does not depend on the choice of numbering vertices. Moreover,

Lemma 3.1.2 If $G \cong G'$, then Spec (G) =Spec (G').

Remark 3.1.3 The converse assertion of Lemma 3.1.2 is not valid, however, it is known that the converse is true for graphs with four or less vertices. In Section 3.6 we show examples of two non-isomorphic graphs whose spectra coincide.

Example 3.1.4 Here are some simple examples.

$$\operatorname{Spec}(\bullet) = \begin{pmatrix} 0\\1 \end{pmatrix}, \quad \operatorname{Spec}(\bullet \bullet \bullet) = \begin{pmatrix} -1 & 1\\1 & 1 \end{pmatrix},$$
$$\operatorname{Spec}(\bullet \bullet \bullet \bullet) = \begin{pmatrix} -\sqrt{2} & 0 & \sqrt{2}\\1 & 1 & 1 \end{pmatrix}, \quad \operatorname{Spec}\left(\bigstar \right) = \begin{pmatrix} -1 & 2\\2 & 1 \end{pmatrix}.$$

Theorem 3.1.5 The spectrum of the path P_n is given by

$$\operatorname{Spec}\left(P_{n}\right) = \begin{pmatrix} 2\cos\frac{\pi}{n+1} & \cdots & 2\cos\frac{k\pi}{n+1} & \cdots & 2\cos\frac{n\pi}{n+1} \\ 1 & \cdots & 1 & \cdots & 1 \end{pmatrix}$$

PROOF. First we find the zeroes of the Chebyshev polynomial of the second kind. By definition,

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \qquad x = \cos\theta.$$

In view of the right-hand side we see easily that $U_n(x) = 0$ if

$$\theta = \frac{k\pi}{n+1}, \qquad k = 1, 2, \dots, n.$$

For these θ , $\cos \theta$ are mutually distinct. Thus

$$x_k = \cos \frac{k\pi}{n+1}, \qquad k = 1, 2, \dots, n,$$
 (3.3)

form n different zeroes of $U_n(x)$. Since $U_n(x)$ is a polynomial of degree n, (3.3) exhaust the zeroes of $U_n(x)$ and each x_k has multiplicity one.

By Theorem 2.4.4 the characteristic polynomial of P_n is given by $U_n(x/2)$. For the spectrum of P_n it is sufficient to find its zeroes. From the above argument we see that the zeroes of $U_n(x/2)$ are

$$\lambda_k = 2\cos\frac{k\pi}{n+1}, \qquad k = 1, 2, \dots, n,$$

each of which is of multiplicity one. This shows the assertion.

3.2 Number of Walks

Let A be the adjacency matrix of a locally finite graph G = (V, E). Then for any m = 1, 2, ... and $x, y \in V$ the matrix element $(A^m)_{xy}$ is defined as usual by

$$(A^m)_{xy} = \sum_{z_1,\dots,z_{m-1} \in V} (A)_{xz_1} (A)_{z_1 z_2} \cdots (A)_{z_{m-1} y}.$$

Note that

$$(A)_{xz_1}(A)_{z_1z_2}\cdots(A)_{z_{m-1}y} = \begin{cases} 1, & \text{if } x \sim z_1 \sim \cdots \sim z_{m-1} \sim y, \\ 0, & \text{otherwise.} \end{cases}$$

Hence $(A^m)_{xy}$ is the number of walks of length *m* connecting *x* and *y*. If the graph *G* is locally finite, $(A^m)_{xy} < \infty$. Therefore, the powers of *A* is well-defined.

We record the above result in the following

Lemma 3.2.1 Let G = (V, E) be a locally finite graph and A its adjacency matrix. Then, for any m = 1, 2, ... and $x, y \in V$, the matrix element $(A^m)_{xy}$ coincides with the number of walks of length m connecting x and y.

Theorem 3.2.2 Let G = (V, E) be a finite graph and $\lambda_1 < \lambda_2 < \cdots < \lambda_s$ exhaust its eigenvalues. For $x, y \in V$ there exist constant numbers $c_i = c_i(x, y)$ $(i = 1, 2, \dots, s)$ such that

$$(A^m)_{xy} = \sum_{i=1}^s c_i(x,y)\lambda_i^m.$$

Here we tacitly understand that $0^0 = 1$ when $\lambda_i = 0$.

PROOF. The first equality is due to Lemma 3.2.1. For the second equality we consider the diagonalization of A. In fact, since A is real symmetric, taking a suitable orthogonal matrix U we have

$$A = U \begin{bmatrix} \lambda_1 E_{m_1} & & \\ & \ddots & \\ & & \lambda_s E_{m_s} \end{bmatrix} U^{-1}.$$

It is then obvious that every element of (A^m) is a linear combination of $\lambda_1^m, \ldots, \lambda_s^m$.

3.3 Maximal Eigenvalue

It is important to know a bound of Spec(G). Let $\lambda_{\max}(G)$ and $\lambda_{\min}(G)$ denote the maximal and minimal eigenvalues of G, respectively. We shall show a simple estimate of $\lambda_{\max}(G)$.

Some statistics concerning the degrees of vertices play an interesting role. We set

$$d_{\max}(G) = \max\{\deg(x) \mid x \in V\},\$$

$$d_{\min}(G) = \min\{\deg(x) \mid x \in V\},\$$

$$\bar{d}(G) = \frac{1}{|V|} \sum_{x \in V} \deg(x).$$

Obviously,

$$d_{\min}(G) \le \bar{d}(G) \le d_{\max}(G).$$

Theorem 3.3.1 For a finite graph G = (V, E) it holds that

$$d_{\min}(G) \le \overline{d}(G) \le \lambda_{\max}(G) \le d_{\max}(G).$$

PROOF. We regard the adjacency matrix A as a linear transformation on \mathbb{C}^n .

1° We prove $\bar{d}(G) \leq \lambda_{\max}(G)$. Let $\boldsymbol{v} = [v_i] \in \mathbf{C}^n$ be the vector whose elements are all one. Then,

$$\langle \boldsymbol{v}, A\boldsymbol{v} \rangle = \sum_{i=1}^{n} \overline{v_i} (A\boldsymbol{v})_i = \sum_{i,j=1}^{n} \overline{v_i} (A)_{ij} v_j = \sum_{i,j=1}^{n} (A)_{ij} = \sum_{i \in V} d(i).$$

Since $\langle \boldsymbol{v}, \boldsymbol{v} \rangle = n = |V|$, we have

$$\frac{\langle \boldsymbol{v}, A\boldsymbol{v} \rangle}{\langle \boldsymbol{v}, \boldsymbol{v} \rangle} = \frac{1}{|V|} \sum_{i \in V} d(i) = \bar{d}(G).$$
(3.4)

On the other hand, it is known from knowledge of linear algebra that

$$\lambda_{\min}(A) \le \frac{\langle \boldsymbol{u}, A\boldsymbol{u} \rangle}{\langle \boldsymbol{u}, \boldsymbol{u} \rangle} \le \lambda_{\max}(A) \quad \text{for all } \boldsymbol{u} \neq \boldsymbol{0}.$$
(3.5)

Combining (3.4) and (3.5), we come to

$$d(G) \le \lambda_{\max}(A) = \lambda_{\max}(G).$$

2° We show $\lambda_{\max}(G) \leq d_{\max}(G)$. Since $\lambda_{\max}(G)$ is real, we may choose its eigenvector $\boldsymbol{u} = [u_i]$ whose elements are all real. Then, for any i we have $(A\boldsymbol{u})_i = \lambda_{\max}u_i$. Multiplying a constant, we may assume that

$$\alpha \equiv \max\{u_i; i = 1, 2, \dots, n\} > 0$$

and choose i_0 such that $u_{i_0} = \alpha$. Then,

$$\lambda_{\max}(G)\alpha = \lambda_{\max}(G)u_{i_0} = (A\boldsymbol{u})_{i_0} = \sum_{i \sim i_0} u_i$$
$$\leq \alpha |\{i \in V \mid i \sim i_0\}| = \alpha d(i_0) \leq \alpha d_{\max}(G),$$

which implies that $\lambda_{\max}(G) \leq d_{\max}(G)$.

Corollary 3.3.2 If G is a regular graph with degree κ , we have $\lambda_{\max}(G) = \kappa$.

PROOF. For a regular graph we have $\bar{d}(G) = d_{\max}(G) = \kappa$.

3.4 Spectral Distribution of a Graph

Definition 3.4.1 Let G be a finite graph with

Spec
$$(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \dots & \lambda_s \\ m_1 & m_2 & \dots & m_s \end{pmatrix}$$
.

The spectral (eigenvalue) distribution of G is a probability measure on \mathbf{R} defined by

$$\mu = \frac{1}{|V|} \sum_{i=1}^{s} m_i \delta_{\lambda_i} \,,$$

where δ_{λ} stands for the delta-measure.

It is sometimes convenient to use the list of eigenvalues of A with multiplicities, say, $\lambda_1, \lambda_2, \ldots, \lambda_n, n = |V|$. Then the spectral distribution is

$$\mu = \frac{1}{n} \sum_{k=1}^{n} \delta_{\lambda_k} \, .$$

Example 3.4.2 The spectral distribution of the path P_n is given by

$$\mu = \frac{1}{n} \sum_{k=1}^{n} \delta_{2\cos\frac{k\pi}{n+1}}$$

Remark 3.4.3 The delta measure δ_{λ} is a Borel probability measure on **R**. For a Borel set $E \subset \mathbf{R}$ we have

$$\delta_{\lambda}(E) = \begin{cases} 1, & \text{if } \lambda \in E, \\ 0, & \text{otherwise} \end{cases}$$

Hence for a continuous function f(x) on **R** we have

$$\int_{-\infty}^{+\infty} f(x)\delta_{\lambda}(dx) = f(\lambda).$$

Definition 3.4.4 Let μ be a probability measure on **R**. The integral, if exists,

$$M_m(\mu) = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots$$
(3.6)

is called the *m*-th moment of μ .

Theorem 3.4.5 Let μ be the spectral distribution of a finite graph G = (V, E). Then,

$$M_m(\mu) = \frac{1}{|V|} \operatorname{Tr} A^m, \qquad m = 1, 2, \dots$$
 (3.7)

PROOF. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A, listed with multiplicities. Then by definition,

$$M_m(\mu) = \int_{-\infty}^{+\infty} x^m \mu(dx) = \frac{1}{n} \sum_{k=1}^n \lambda_k^m$$

Since $\lambda_1^m, \ldots, \lambda_n^m$ is the eigenvalues of A^m with multiplicities, their sum coincides with the trace of A^m . Hence, (3.7) follows.

Lemma 3.4.6 Let A be the adjacency matrix of a finite graph G = (V, E).

- (1) $\operatorname{Tr} A = 0.$
- (2) $\operatorname{Tr}(A^2) = 2|E|.$
- (3) $\operatorname{Tr}(A^3) = 6 \triangle$.

PROOF. We show only (3). By definition

$$\operatorname{Tr}(A^{3}) = \sum_{x,y,z \in V} (A)_{xy}(A)_{yz}(A)_{zx} = |\{(x,y,z) \in V^{3} ; x \sim y \sim z \sim x\}| = 6\Delta.$$

The most basic characteristics of a spectral distribution are the mean and the variance, which are defined by

mean
$$(\mu) = M_1(\mu) = \int_{-\infty}^{+\infty} x\mu(dx),$$

var $(\mu) = M_2(\mu) - M_1(\mu)^2 = \int_{-\infty}^{+\infty} (x - \text{mean}\,(\mu))^2 \mu(dx).$

Proposition 3.4.7 Let μ be the spectral distribution of a finite graph G = (V, E). Then,

mean
$$(\mu) = 0$$
, var $(\mu) = 2 \frac{|E|}{|V|}$.

3.5 Asymptotic Spectral Distributions of P_n and K_n

3.5.1 P_n as $n \to \infty$

The spectral distribution of P_n is

$$\mu_n = \frac{1}{n} \sum_{k=1}^n \delta_{2\cos\frac{k\pi}{n+1}} \,,$$

see Example 3.4.2. Let f(x) be a bounded continuous function. The we have

$$\int_{-\infty}^{+\infty} f(x)\mu_n(dx) = \frac{1}{n} \sum_{k=1}^n f\left(2\cos\frac{k\pi}{n+1}\right) \to \int_0^1 f(2\cos\pi t)dt, \quad \text{as } n \to \infty,$$

which follows by the definition of Riemann integral. By change of variable, one gets

$$\int_0^1 f(2\cos\pi t)dt = \int_{-2}^2 f(x) \,\frac{dx}{\pi\sqrt{4-x^2}}$$

Consequently,

$$\lim_{n \to \infty} \int_{-\infty}^{+\infty} f(x)\mu_n(dx) = \int_{-2}^2 f(x) \, \frac{dx}{\pi\sqrt{4-x^2}}, \qquad f \in C_b(\mathbf{R}), \tag{3.8}$$

where $C_b(\mathbf{R})$ denotes the space of bounded continuous function on \mathbf{R} .

It is easy to see that

$$\frac{dx}{\pi\sqrt{4-x^2}}\,\chi_{(-2,2)}(x)dx$$

is a probability measure on \mathbf{R} . We call it the *arcsine law* with variance 2. Then from the limit formula (3.8) we state the following

Proposition 3.5.1 The spectral distribution of P_n converges weakly to the arcsine law with variance 2.

3.5.2 K_n as $n \to \infty$

The spectral distribution of K_n is

$$\mu_n = \frac{1}{n} \,\delta_{n-1} + \frac{n-1}{n} \,\delta_{-1} \,.$$

In a similar manner as in Section 3.5.1 we have

$$\int_{-\infty}^{+\infty} f(x)\mu_n(dx) = \frac{1}{n} f(n-1) + \frac{n-1}{n} f(-1) \to f(-1), \quad \text{as } n \to \infty.$$

Since

$$f(-1) = \int_{-\infty}^{+\infty} f(x)\delta_{-1}(dx)$$

and δ_{-1} is a probability measure, we may state that the spectral distribution of K_n converges weakly to δ_{-1} . However, notice that

mean
$$(\mu_n) = 0$$
, var $(\mu_n) = 2 \frac{|E|}{|V|} = n - 1$,

and

$$mean(\delta_{-1}) = -1, \quad var(\delta_{-1}) = 0$$

Thus, it is hardly to say that the limit measure δ_{-1} reflects basic statistical properties of μ_n for a large n.

The above unconfort was caused by $\operatorname{var}(\mu_n) \to \infty$ as $n \to \infty$. In order to capture a reasonable limit measure it is necessary to handle a normalized measure. In general, for a probability measure μ with mean mean $(\mu) = m$ and variance $\operatorname{var}(\mu) = \sigma^2$, the normalization is defined by

$$\int_{-\infty}^{+\infty} f(x)\bar{\mu}(dx) = \int_{-\infty}^{+\infty} f\left(\frac{x-m}{\sigma}\right)\mu(dx).$$

Then mean $(\bar{\mu}) = 0$ and var $(\bar{\mu}) = 1$.

Proposition 3.5.2 The normalized spectral distribution of K_n converges weakly to δ_0 .

PROOF. Let f(x) be a bounded continuous function on **R**. We have

$$\int_{-\infty}^{+\infty} f(x)\bar{\mu}_n(dx) = \int_{-\infty}^{+\infty} f\left(\frac{x}{\sqrt{n-1}}\right)\mu_n(dx)$$
$$= \frac{1}{n}f\left(\frac{n-1}{\sqrt{n-1}}\right) + \frac{n-1}{n}f\left(\frac{-1}{\sqrt{n-1}}\right)$$
$$\to f(0), \quad \text{as } n \to \infty.$$

This completes the proof.

In Section 3.5.1, for the asymptotic spectral distribution of P_n we did not take the normalization. The normalization yields essentially nothing new thanks to the fact that

mean
$$(\mu_n) = 0$$
, var $(\mu_n) = 2 \frac{|E|}{|V|} = \frac{2(n-1)}{n}$.

Namely, the variance of μ_n stays bounded by 2 as $n \to \infty$.

3.6 Isospectral (Cospectral) Graphs

We show a pair of non-isomorphic graphs that have the same spectra.

Example 3.6.1 $\varphi(x) = x^5 - 4x^3 = x^3(x-2)(x+2).$



Example 3.6.2 (Baker)

$$\varphi(x) = x^6 - 7x^4 - 4x^3 + 7x^2 + 4x - 1$$

= $(x - 1)(x + 1)^2(x^3 - x^2 - 5x + 1)$



Example 3.6.3 (Collatz–Sinogowitz) $\varphi(x) = x^8 - 7x^6 + 9x^4$



For more information see e.g.,

- [6] D. M. Cvetković, M. Doob and H. Sachs: Spectra of Graphs: Theory and Applications (3rd rev. enl. ed.), New York, Wiley, 1998.
- [7] L. Collatz and U. Sinogowitz: Spektren endlicher Grafen, Abh. Math. Sem. Univ. Hamburg 21 (1957), 63–77.
- [8] C. D. Godsil and B. D. McKay: Constructing cospectral graphs, Aeq. Math. 25 (1982), 257–268.

3.7 Exercises

- (1) Let C_n be a cycle of *n* vertices. Find Spec (C_n)
- (2) Let μ_n be the spectral distribution of C_n . Study the asymptotics of μ_n as $n \to \infty$.
- (3) Using Theorem 3.1.5, prove the formula:

$$\prod_{k=1}^{m} 2\cos\frac{k\pi}{2m+1} = 1.$$

4 Adjacency Algebras

4.1 Adjacency Algebras

Let A be the adjacency matrix of a locally finite graph G = (V, E). In Section 3.2 we showed that every matrix element of A^m (m = 1, 2, ...) is defined and finite, so we may form their linear combination. Let $\mathcal{A}(G)$ denote the set of linear combinations of $E, A, A^2, ...$ with complex coefficients.

Equipped with the usual operations, $\mathcal{A}(G)$ becomes a commutative algebra over **C** with the multiplication identity *E*. Moreover, we define the involution by

 $(c_0E + c_1A + c_2A^2 + \dots + c_mA^m)^* = \bar{c_0}E + \bar{c_1}A + \bar{c_2}A^2 + \dots + \bar{c_m}A^m$

so that $\mathcal{A}(G)$ becomes a *-algebra.

Definition 4.1.1 The above $\mathcal{A}(G)$ is called the *adjacency algebra* of G.

Proposition 4.1.2 If G is a finite graph, dim $\mathcal{A}(G)$ coincides with the number of different eigenvalues of A.

PROOF. Let $\lambda_1 < \cdots < \lambda_s$ be the different eigenvalues of A. Then, by a suitable orthogonal matrix U we have

$$U^{-1}AU = \begin{bmatrix} \lambda_1 E_{m_1} & & \\ & \ddots & \\ & & \lambda_s E_{m_s} \end{bmatrix} \equiv D.$$

We see that $\{E, D, D^2, \dots, D^{s-1}\}$ is linearly independent, but $\{E, D, D^2, \dots, D^{s-1}, D^s\}$ is not. In fact,

$$(D - \lambda_1 E) \cdots (D - \lambda_s E) = O$$

Therefore, the algebra $U^{-1}\mathcal{A}U$ is of dimension s, so is $\mathcal{A}(G)$.

Proposition 4.1.3 For a connected finite graph G = (V, E) we have

$$\dim \mathcal{A}(G) \ge \operatorname{diam}(G) + 1.$$

PROOF. For simplicity put diam (G) = d. If d = 0, we have |V| = 1 and dim $\mathcal{A}(G) = 1$ so the assertion is clear. Assume that $d \ge 1$. By definition of the diameter there exists a pair of verices $x, y \in V$ such that $\partial(x, y) = d$. Choose one path of length d connecting x, y, say,

$$x = x_0 \sim x_1 \sim \cdots \sim x_k \sim x_{k+1} \sim \cdots \sim x_d = y.$$

In this case, x_0, x_1, \ldots, x_d are all distinct and $\partial(x, x_k) = k$ $(0 \le k \le d)$. In particular, there is no walk of length $\le k - 1$ connecting x and x_k . Hence

$$(A^m)_{xx_k} = 0, \quad 0 \le m \le k - 1; \qquad (A^k)_{xx_k} \ne 0.$$

Then we see by induction on k that $\{E = A^0, A, A^2, \ldots, A^k\}$ $(1 \le k \le d)$ is linearly independent. Consequently, $\mathcal{A}(G)$ contains a linearly independent subset consisting of d+1 elements, so that dim $\mathcal{A}(G) \ge d+1$.

Corollary 4.1.4 A connected finite graph G = (V, E) has at least diam (G) + 1 different eigenvalues.

PROOF. By combining Propositions 4.1.2 and 4.1.3.

Example 4.1.5 (1) K_n $(n \ge 2)$.

(number of different eigenvalues) = 2,
$$\operatorname{diam}(K_n) = 1$$
.

(2) $P_n \ (n \ge 1)$.

(number of different eigenvalues) = n, diam $(P_n) = n - 1$.

(3) G as below. $\varphi_G(x) = x^2(x+2)(x^2-2x-4)$



(number of different eigenvalues) = 4, diam (G) = 2.

4.2 Distance-Regular Graphs (DRGs)

Let G = (V, E) be a connected graph and fix a vertex $o \in V$ as an origin (root). We set

$$V_n = \{ x \in V ; \ \partial(x, o) = n \}, \qquad n = 0, 1, 2, \dots$$

Obviously,

$$V_0 = \{o\}, \qquad V_1 = \{x \in V ; x \sim o\}.$$

If G is a finite graph, there exists $m_0 \ge 1$ such that $V_{m_0-1} \ne \emptyset$ and $V_{m_0} = \emptyset$. If G is an infinite, locally finite graph, $V_n \ne \emptyset$ for all $n \ge 0$. In any case we have a partition of the vertices:

$$V = \bigcup_{n=0}^{\infty} V_n \tag{4.1}$$

which is called the *stratification* of the graph G with respect to the origin $o \in V$.

Lemma 4.2.1 Let G be a connected, locally finite graph and let (4.1) be a stratification. If $x \in V_n$ and $y \sim x$, we have $y \in V_{n+1} \cup V_n \cup V_{n-1}$.

PROOF. Obvious.

Given a stratification, for $x \in V_n$ we define

$$\omega_{+}(x) = \{ y \in V_{n+1} ; y \sim x \},
\omega_{\circ}(x) = \{ y \in V_{n} ; y \sim x \},
\omega_{-}(x) = \{ y \in V_{n-1} ; y \sim x \}$$



Figure 4.1: Stratification and $\omega_{\epsilon}(x)$

It is convenient to write

$$\omega_{\epsilon}(x) = \{ y \in V_{n+\epsilon} ; y \sim x \}, \qquad \epsilon \in \{+, -, \circ\},$$

where ϵ takes the values +1, -1, 0 according to $\epsilon = +, -, \circ$. Note also that

$$\deg(x) = \omega_+(x) + \omega_\circ(x) + \omega_-(x), \qquad x \in V.$$

Definition 4.2.2 A connected graph G = (V, E) is called *distance-regular* if, for any stratification of G, the functions $\omega_{\epsilon} : V \to \{0, 1, 2, ...\}$ ($\epsilon \in \{+, -, \circ\}$) are constant on V_n , and the constants are independent of the choice of stratification. In that case we put

$$b_n = \omega_+(x), \qquad c_n = \omega_-(x), \qquad a_n = \omega_\circ(x),$$

by taking $x \in V_n$.

It is obvious that

$$a_0 = c_0 = 0,$$
 $b_0 = \deg(x),$ $x \in V_0.$

Since any vertex x may be chosen as an origin for stratification, $\deg(x) = b_0$ for all $x \in V$. That is, a distace-regular graph is regular with degree b_0 . Therefore,

$$a_n + b_n + c_n = b_0, \qquad n = 1, 2, \dots$$

Lemma 4.2.3 If G is a finite DRG, letting d = diam(G), we have

$$V = \bigcup_{n=0}^{d} V_n, \qquad V_0, V_1, \dots, V_d \neq \emptyset.$$
(4.2)

If G is an infinite DRG, $V_n \neq \emptyset$ for all n = 0, 1, 2, ...

PROOF. By definition, there is a path of length d. Taking one of the end vertex as an origin, the associated stratification satisfies conditions in (4.2). Then, we have

$$b_0 > 0, \dots, b_{d-1} > 0, b_d = 0.$$
 (4.3)

Let $o \in V$ be an aritrary vertex and take $v \in V$ such that

$$\partial(o, v) = \max\{\partial(o, x) \, ; \, x \in V\} \equiv p$$

Then $p \leq d$ and the associated stratification is

$$V = \bigcup_{k=0}^{p} V'_{k}, \qquad V'_{0}, V'_{1}, \dots, V'_{p} \neq \emptyset.$$

Then,

 $b_0 > 0, \dots, b_{p-1} > 0, b_p = 0.$ (4.4)

In order that (4.3) and (4.4) are consistent, we have p = d.

Corollary 4.2.4 In a finite distance-regular graph, every vertex is an end vertex of a diameter.

Definition 4.2.5 For a finite distance-regular graph G, the table of associated constant numbers

$$\begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_d \\ a_0 & a_1 & a_2 & \cdots & a_d \\ b_0 & b_1 & b_2 & \cdots & b_d \end{pmatrix}$$

is called the *intersection array* of G. If G is infinite, the array becomes infinite.

Since $a_n + b_n + c_n = b_0$ is constant, the row of a_0, a_1, \ldots may be omitted. Note that

$$c_0 = 0, \quad c_1 > 0, \quad \cdots, \quad c_{d-1} > 0, \quad c_d > 0,$$

 $b_0 > 0, \quad b_1 > 0, \quad \cdots, \quad b_{d-1} > 0, \quad b_d = 0.$

Example 4.2.6 (1) The cheapest examples are C_n $(n \ge 3)$, K_n $(n \ge 1)$, and $K_{n,n}$ $(n \ge 1)$. (2) The Petersen graph is distance-regular.

(3) A homogeneous tree of degree κ , T_{κ} , is distance-regular.

(4) P_n $(n \ge 3)$ is not distance-regular (sine it is not regular).

(5) \mathbf{Z}^2 is not distance-regular.

Definition 4.2.7 A connected graph is called *distance-transitive* if, for any $x, x', y, y' \in V$ with $\partial(x, y) = \partial(x', y')$ there exists $\alpha \in \text{Aut}(G)$ such that $\alpha(x) = x'$ and $\alpha(y) = y'$.

Proposition 4.2.8 A distance-transitive graph is distance-regular.

In fact, (1)-(3) in Example 4.2.6 are all distance-transitive. The converse of Proposition 4.2.8 is not valid, for examples see Godsil-Royle [9: p.69], Brouwer et al. [10: p.136].

4.3 Adjacency Algebras of Distance-Regular Graphs

Definition 4.3.1 Let G = (V, E) be a connected graph. For k = 0, 1, 2, ... we define a matrix $A^{(k)}$ indexed by $V \times V$ by

$$(A^{(k)})_{xy} = \begin{cases} 1, & \text{if } \partial(x,y) = k, \\ 0, & \text{otherwise} \end{cases}$$

This matrix is called the k-th distance matrix.

Obviously,

$$A^{(0)} = E$$
 (identity), $A^{(1)} = A$ (adjacency matrix)

and we have

$$\sum_{k=0}^{\infty} A^{(k)} = J, \qquad J \text{ is the matrix whose elements are all one.}$$

Lemma 4.3.2 Let G be a distance-regular graph with the intersection array

$$\begin{pmatrix} c_0 & c_1 & c_2 & \cdots \\ a_0 & a_1 & a_2 & \cdots \\ b_0 & b_1 & b_2 & \cdots \end{pmatrix}$$

Then,

$$AA^{(k)} = c_{k+1}A^{(k+1)} + a_kA^{(k)} + b_{k-1}A^{(k-1)}, \qquad k = 0, 1, 2, \dots$$
(4.5)

Here we understand that $A^{(-1)} = O$ and $A^{(d+1)} = O$ for $d = \operatorname{diam}(G) < \infty$.

PROOF. For k = 0 the equality (4.5) is obvious. Let $k \ge 1$. Let $x, y \in V$ and set $n = \partial(x, y)$. Then, by definition

$$(AA^{(k)})_{xy} = \sum_{z \in V} (A)_{xz} (A^{(k)})_{zy} = |\{z \in V ; \ \partial(z, x) = 1, \ \partial(z, y) = k\}|.$$

It is obvious by the triangle inequality,

$$\{z \in V \, ; \, \partial(z, x) = 1, \, \partial(z, y) = k\} = \emptyset$$

unless $k - 1 \le n \le k + 1$. Namely,

$$(AA^{(k)})_{xy} = 0 \qquad \text{unless } k - 1 \le n \le k + 1.$$

Assume that $k-1 \leq n \leq k+1$. Then, by definition of the intersection array, we have

$$|\{z \in V; \, \partial(z, x) = 1, \, \partial(z, y) = k\}| = \begin{cases} c_n, & k = n - 1, \\ a_n, & k = n, \\ b_n, & k = n + 1. \end{cases}$$

Thus,

$$(AA^{(k)})_{xy} = \begin{cases} c_{k+1}, & \partial(x,y) = k+1, \\ a_k, & \partial(x,y) = k, \\ b_{k-1}, & \partial(x,y) = k-1. \end{cases}$$

This completes the proof.

Lemma 4.3.3 For k = 0, 1, 2, ..., d, $A^{(k)}$ is a polynomial in A with degree k.

PROOF. For k = 0, 1 the assertion is apparently true. In fact,

$$A^{(0)} = f_0(A),$$
 $f_0(x) = 1,$
 $A^{(1)} = f_1(A),$ $f_1(x) = x.$

It follows from Lemma 4.3.2 that

$$A^{(k)} = f_k(A), \qquad f_k(x) = \frac{1}{c_k} \left(x - a_{k-1} \right) f_{k-1}(x) - \frac{b_{k-2}}{c_k} f_{k-2}(x)$$

for $k = 2, 3, \ldots, d$. Note that $c_1 > 0, \cdots, c_d > 0$.

Theorem 4.3.4 Let G be a distance-regular graph. Then the adjacency algebra $\mathcal{A}(G)$ coincides with the linear span of $\{A^{(0)}, A^{(1)}, \ldots\}$, which are linearly independent. If G is a finite distance-regular graph, dim $\mathcal{A}(G) = \text{diam}(G) + 1$ and A has diam (G) + 1 distinct eigenvalues.

PROOF. It follows from Lemma 4.3.3 that the adjacency algebra $\mathcal{A}(G)$ contains the linear span of $\{A^{(0)}, A^{(1)}, \ldots\}$. On the other hand, since

$$A^{(k)} = f_k(A) = \beta_k A^k + \dots, \qquad \beta_k > 0,$$

we see that A^k is a linear combination of $A^{(0)}, A^{(1)}, \ldots, A^{(k)}$. Therefore, $\mathcal{A}(G)$ is contained in the linear span of $\{A^{(0)}, A^{(1)}, \ldots\}$.

The second half is obvious because the distance matrices $\{A^{(0)}, A^{(1)}, \ldots\}$ are linearly independent.

Theorem 4.3.5 (Linearization formula) For $i, j, k \in \{0, 1, 2, ..., d\}$ there exists a unique constant p_{ij}^k such that

$$A^{(i)}A^{(j)} = \sum_{k=0}^{d} p_{ij}^{k} A^{(k)} \qquad i, j \in \{0, 1, 2, \dots, d\}.$$
(4.6)

Moreover, for $x, y \in V$ with $\partial(x, y) = k$,

$$|\{z \in V \, ; \, \partial(z, x) = i, \, \partial(z, y) = j\}|$$

does not depend on the choice of x, y but depends on k, and coincides with p_{ij}^k .

4.4. EXERCISES

PROOF. The first half is obvious by Theorem 4.3.4. Let $x, y \in V$ with $\partial(x, y) = l$. Let us observe the matrix element of (4.6). From the left-hand side we get

$$(A^{(i)}A^{(j)})_{xy} = \sum_{z \in V} (A^{(i)})_{xz} (A^{(j)})_{zy} = |\{z \in V ; \, \partial(z, x) = i, \, \partial(y, z) = j\}|$$

On the other hand,

$$\left(\sum_{k=0}^d p_{ij}^k A^{(k)}\right)_{xy} = p_{ij}^l \,,$$

which is constant for all $x, y \in V$ with $\partial(x, y) = l$. Therefore, for such a pair x, y we have

$$|\{z \in V \, ; \, \partial(z,x) = i, \, \partial(y,z) = j\}| = p_{ij}^l$$

as desired.

Definition 4.3.6 The constant numbers $\{p_{ij}^k\}$ are called the *intersection numbers* of a distance-regular graph G.

The intersection numbers satisfies:

- (1) $p_{1n}^{n-1} = b_{n-1}, \quad p_{1n}^n = a_n, \quad p_{1n}^{n+1} = c_{n+1}.$ (2) $p_{ij}^k = 0$ unless $|i - j| \le k \le i + j.$ (3) $p_{ij}^k = p_{ji}^k.$
- (4) $p_{00}^0 = 1$, $p_{0i}^0 = p_{i0}^0 = 0$ for $i \ge 1$.

Remark 4.3.7 In some of the literature, a distance-regular graph is defined to be a connected graph for which the set of constants $\{p_{ij}^k\}$, where $i, j, k \in \{0, 1, 2, ...\}$,

$$p_{ij}^k = |\{z \in V; \, \partial(z, x) = i, \, \partial(y, z) = j\}|$$

is independent of the choice of $x, y \in V$ with $\partial(x, y) = k$. This condition is seemingly stronger than that of our definition (Definition 4.2.2) as is seen in (1) above; however, they are equivalent.

4.4 Exercises

(1) Verify that the Petersen graph is distance-regular and find its intersection array.

Ans. $\begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 2 \\ 3 & 2 & 0 \end{pmatrix}$

(2) Verify that the one-dimensional integer lattice \mathbb{Z} is distance-regular and find its intersection array.



(3) Define a polynomial $T_n(x)$ by $T_n(\cos \theta) = \cos n\theta$ and set

$$\tilde{T}_0(x) = T_0(x) = 1, \qquad \tilde{T}_n(x) = 2T_n\left(\frac{x}{2}\right), \quad n \ge 1.$$

Let A and $A^{(k)}$ be the adjacency matrix and the k-th distance matrix of \mathbb{Z} , respectively. Show that $A^{(k)} = \tilde{T}_k(A)$. ({ $T_n(x)$ } are calle the *Chebyshev polynomial of the first kind.*)

References

- [9] C. Godsil and G. Royle: Algebraic Graph Theory, Springer, 2001.
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5 Spectral Distributions of Distance-Regular Graphs

5.1 Quantum Decomposition

Let G = (V, E) be a connected graph. Fix an origin $o \in V$ we consider the stratification:

$$V = \bigcup_{n=0}^{\infty} V_n, \qquad V_n = \{ x \in V ; \ \partial(x, o) = n \}.$$

Let A be the adjacency matrix.

We define three matrices A^{ϵ} as follows: Let $x \in V_n$.

$$(A^+)_{yx} = \begin{cases} 1, & \text{if } y \sim x \text{ and } y \in V_{n+1}, \\ 0, & \text{otherwise}, \end{cases}$$
$$(A^\circ)_{yx} = \begin{cases} 1, & \text{if } y \sim x \text{ and } y \in V_n, \\ 0, & \text{otherwise}, \end{cases}$$
$$(A^-)_{yx} = \begin{cases} 1, & \text{if } y \sim x \text{ and } y \in V_{n-1}, \\ 0, & \text{otherwise}, \end{cases}$$

It is convenient to unify the above in the following form:

$$(A^{\epsilon})_{yx} = \begin{cases} 1, & \text{if } y \sim x \text{ and } y \in V_{n+\epsilon}, \\ 0, & \text{otherwise,} \end{cases} \quad \epsilon \in \{+, -, \circ\}.$$



Figure 5.1: Quantum decomposition of the adjacency matrix

Lemma 5.1.1 (1) $A = A^+ + A^- + A^\circ$.

- (2) $(A^+)^* = A^-$ and $(A^-)^* = A^+$.
- (3) $(A^{\circ})^* = A.$

PROOF. Easy.

Definition 5.1.2 We call $A = A^+ + A^- + A^\circ$ the quantum decomposition of the adjacency matrix with respect to the origin $o \in V$. Each A^ϵ is called a quantum component.

Example 5.1.3 (1) P_n .



(2) P_7 with the origin o as illustrated below.



$$A = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & 1 & 0 & 1 & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & & & & & \\ 1 & 0 & & & & \\ & & 1 & 0 & 1 & & \\ & & & & 0 & 1 & \\ & & & & & 0 & 1 \\ & & & & & 0 & 1 \\ & & & & & 0 & 1 \\ & & & & & 0 & 1 \\ & & & & & & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 & & & & \\ 0 & 1 & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 1 & 0 & \\ & & & 1 & 0 \end{bmatrix}$$

5.2 Interacting Fock Spaces (IFSs)

We put

 $C(V) = \{ f : V \to \mathbf{C} ; \text{ supported by a finite subset of } V \}.$

Equipped with the usual operation, C(V) becomes a complex vector space. We define the inner product by

$$\langle f,g\rangle = \sum_{x\in V} \overline{f(x)} g(x).$$

With each $x \in V$ we associate a function $e_x \in C(V)$ defined by

$$e_x(y) = \begin{cases} 1, & \text{if } y = x, \\ 0, & \text{otherwise} \end{cases}$$

Then $\{e_x\}$ becomes a basis of C(V) satisfying $\langle e_x, e_y \rangle = \delta_{xy}$.

Let $V = \bigcup_{n=0}^{\infty} V_n$ be a stratification. Then we define

$$\Phi_n = \frac{1}{\sqrt{|V_n|}} \sum_{x \in V_n} e_x$$

By definition, $\Phi_0 = e_o$. We note that

$$\langle \Phi_m, \Phi_n \rangle = \delta_{mn}$$

Let $\Gamma = \Gamma(G, o)$ denote the subspace of C(V) spanned by Φ_0, Φ_1, \ldots

A matrix T indexed by $V \times V$ acts on C(V) from the left by the usual matrix multiplication. Note that

$$\langle f, Tg \rangle = \langle T^*f, g \rangle, \qquad f, g \in C(V)$$

We are interested in the actions of the quantum components of the adjacency matrix: $A = A^+ + A^- + A^\circ$.

Lemma 5.2.1 For $x \in V_n$,

$$A^{\epsilon}e_x = \sum_{y \in V_{n+\epsilon}, y \sim x} e_y, \qquad \epsilon \in \{+, -, \circ\}.$$

Lemma 5.2.2

$$A^{\epsilon}\Phi_n = \frac{1}{\sqrt{|V_n|}} \sum_{y \in V_{n+\epsilon}} |\omega_{-\epsilon}(y)| e_y$$
(5.1)

PROOF. Let us consider A^+ . By definition

$$\sqrt{|V_n|}A^+\Phi_n = \sum_{x \in V_n} A^+ e_x = \sum_{y \in V_{n+1}} |\omega_-(y)|e_y,$$

which prooves the assertion.

We see from (5.1) that $A^{\epsilon}\Phi_n$ is not necessarily a constant multiple of $\Phi_{n+\epsilon}$, in other words, Γ is not necessarily closed under the actions of the quantum components. The quantum probabilistic approach is useful in the case where

(i) Γ is closed under the actions of the quantum components;

(ii) Γ is asymptotically closed under the actions of the quantum components.

Here we discuss typical examples for (i).

Theorem 5.2.3 Let G be a distance-regular graph with the intersection array:

$$\begin{pmatrix} c_0 & c_1 & c_2 & \cdots \\ a_0 & a_1 & a_2 & \cdots \\ b_0 & b_1 & b_2 & \cdots \end{pmatrix}.$$

Fix an origin $o \in V$, we consider the stratification of G, the unit vectors $\Phi_0 = e_o, \Phi_1, \Phi_2, \ldots$, the linear space $\Gamma = \Gamma(G, o)$, and the quantum decomposition of the adjacency matrix $A = A^+ + A^- + A^\circ$. Then, Γ is invariant under the actions of the quantum components A^ϵ . Moreover,

$$A^{+}\Phi_{n} = \sqrt{\omega_{n+1}} \Phi_{n+1}, \quad n = 0, 1, \dots,$$
(5.2)

$$A^{-}\Phi_{0} = 0, \quad A^{-}\Phi_{n} = \sqrt{\omega_{n} \Phi_{n-1}}, \quad n = 1, 2, \dots,$$
 (5.3)

$$A^{\circ}\Phi_n = \alpha_{n+1}\Phi_n, \quad n = 0, 1, 2, \dots,$$
 (5.4)

where

$$\omega_n = b_{n-1}c_n, \qquad \alpha_n = a_{n-1}, \qquad n = 1, 2, \dots$$

PROOF. We continue the calculation of (5.1). Since G is distance-regular, we know that for $y \in V_{n+\epsilon}$,

$$|\omega_{-\epsilon}(y)| = \begin{cases} c_{n+1}, & \text{if } \epsilon = +, \\ a_n, & \text{if } \epsilon = \circ, \\ b_{n-1}, & \text{if } \epsilon = -. \end{cases}$$

Then, for $\epsilon = +$ we have

$$A^{+}\Phi_{n} = \frac{1}{\sqrt{|V_{n}|}} \sum_{y \in V_{n+1}} c_{n+1}e_{y} = c_{n+1} \frac{\sqrt{|V_{n+1}|}}{\sqrt{|V_{n}|}} \Phi_{n+1}.$$
(5.5)

Similarly,

$$A^{-}\Phi_{n} = \frac{1}{\sqrt{|V_{n}|}} \sum_{y \in V_{n-1}} b_{n-1}e_{y} = b_{n-1} \frac{\sqrt{|V_{n-1}|}}{\sqrt{|V_{n}|}} \Phi_{n-1}$$
(5.6)

and

$$A^{\circ}\Phi_{n} = \frac{1}{\sqrt{|V_{n}|}} \sum_{y \in V_{n}} a_{n}e_{y} = a_{n}\Phi_{n}.$$
(5.7)

Now (5.4) is obvious from (5.6). We note that

$$b_n |V_n| = c_{n+1} |V_{n+1}|,$$

wich counts the number of edges between two strata V_n and V_{n+1} . Then, the coefficient on the right-hand side of (5.5) becomes

$$c_{n+1} \frac{\sqrt{|V_{n+1}|}}{\sqrt{|V_n|}} = c_{n+1} \sqrt{\frac{b_n}{c_{n+1}}} = \sqrt{b_n c_{n+1}} = \sqrt{\omega_{n+1}} \,.$$

Similarly, for (5.6) we have

$$b_{n-1} \frac{\sqrt{|V_{n-1}|}}{\sqrt{|V_n|}} = b_{n-1} \sqrt{\frac{c_n}{b_{n-1}}} = \sqrt{b_{n-1}c_n} = \sqrt{\omega_n}$$

These show that (5.2) and (5.3).

Definition 5.2.4 A real sequence $\{\omega_n\}_{n=1}^{\infty}$ is called a *Jacobi sequence* if

- (i) [infinite type] $\omega_n > 0$ for all $n \ge 1$; or
- (ii) [finite type] there exists $m_0 \ge 1$ such that $\omega_1 > 0$, $\omega_2 > 0$, ..., $\omega_{m_0-1} > 0$, $\omega_{m_0} = \omega_{m_0+1} = \cdots = 0$.

By definition (0, 0, ...) is a Jacobi sequence $(m_0 = 1)$.

Given a Jacobi sequence $\{\omega_n\}$, we consider a Hilbert space Γ as follows: If $\{\omega_n\}$ is of infinite type, let Γ be an infinite dimensional Hilbert space with an orthonormal basis $\{\Phi_0, \Phi_1, \ldots\}$. If $\{\omega_n\}$ is of finite type, let Γ be an m_0 -dimensional Hilbert space with an orthonormal basis $\{\Phi_0, \Phi_1, \ldots, \Phi_{m_0-1}\}$. We call Φ_0 the vacuum vector.

We next define linear operators B^{\pm} on Γ by

$$B^{+}\Phi_{n} = \sqrt{\omega_{n+1}} \Phi_{n+1}, \quad n = 0, 1, \dots,$$
(5.8)

$$B^{-}\Phi_{0} = 0, \quad B^{-}\Phi_{n} = \sqrt{\omega_{n}} \Phi_{n-1}, \quad n = 1, 2, \dots,$$
 (5.9)

where we understand $B^+\Phi_{m_0-1} = 0$ when $\{\omega_n\}$ is of finite type.

Definition 5.2.5 Let $\{\omega_n\}$ be a Jacobi sequence. Let Γ be a Hilbert space constructed from it and B^{\pm} linear operators defined as above. The quadraple $(\Gamma, \{\omega_n\}, B^+, B^-)$ is called an *interaction Fock space* associated with a Jacobi sequence $\{\omega_n\}$. We call B^- the *annihilation operator* and B^+ the *creation operator*.

With these notation Theorem 5.2.3 is rephrased as follows.

Theorem 5.2.6 Let G be a distance-regular graph with the intersection array:

$$\begin{pmatrix} c_0 & c_1 & c_2 & \cdots \\ a_0 & a_1 & a_2 & \cdots \\ b_0 & b_1 & b_2 & \cdots \end{pmatrix}.$$

Fix an origin $o \in V$, we consider the stratification of G, the unit vectors $\Phi_0 = e_o, \Phi_1, \Phi_2, \ldots$, the linear space $\Gamma = \Gamma(G, o)$, and the quantum decomposition of the adjacency matrix $A = A^+ + A^- + A^\circ$. Set $\omega_n = b_{n-1}c_n$ for $n = 1, 2, \ldots$. Then, $(\Gamma, \{\omega_n\}, A^+, A^-)$ is an interacting Fock space.

Figure 5.2: Interaction Fock space

5.3 Orthogonal Polynomials

Let μ be a probability measure on **R** satisfying

$$\int_{-\infty}^{+\infty} |x|^m \mu(dx) < \infty, \qquad m = 1, 2, \dots$$

Let $\mathfrak{P}_{fm}(\mathbf{R})$ be the set of such probability measures.

Definition 5.3.1 For $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$,

$$M_m = M_m(\mu) = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots$$

is called the *m*-th moment of μ .

We denote the inner product of $L^2({\bf R},\mu)$ by

$$\langle f,g\rangle = \int_{-\infty}^{+\infty} \overline{f(x)} g(x) \mu(dx).$$

Now we define a sequence of polynomials $P_0(x), P_1(x), \ldots$ by the following recursive formula:

$$P_{0} = 1, \qquad P_{1} = x - \frac{\langle P_{0}, x \rangle}{\langle P_{0}, P_{0} \rangle} P_{0}, \qquad P_{2} = x^{2} - \frac{\langle P_{0}, x^{2} \rangle}{\langle P_{0}, P_{0} \rangle} P_{0} - \frac{\langle P_{1}, x^{2} \rangle}{\langle P_{1}, P_{1} \rangle} P_{1}, \qquad \dots,$$
$$P_{n} = x^{n} - \sum_{k=0}^{n-1} \frac{\langle P_{k}, x^{n} \rangle}{\langle P_{k}, P_{k} \rangle} P_{k}.$$

This is the co-called Gram-Schmidt orthogonalization. Then,

$$P_n(x) = x^n + \cdots, \qquad \langle P_m, P_n \rangle = 0 \quad \text{for } m \neq n.$$

We call $\{P_n\}$ the orthogonal polynomials associated with μ .

The procedure of forming the orthogonal polynomials stops at the m_0 step if

$$\langle P_0, P_0 \rangle > 0, \quad \dots, \quad \langle P_{m_0-1}, P_{m_0-1} \rangle > 0, \quad \langle P_{m_0}, P_{m_0} \rangle = 0$$

happens. In that case the orthogonal polynomials consists of $P_0(x), P_1(x), \ldots, P_{m_0-1}(x)$. This happens if and only if supp (μ) consists of exactly m_0 points, i.e., μ is a sum of delta measures at different m_0 points with positive coefficients.

Theorem 5.3.2 (The three-term recurrence relation) Let $\{P_n(x)\}_{n=0}^{\infty}$ be the orthogonal polynomials associated with $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$. Then there exist a pair of sequences $\{\alpha_n\}_{n=1}^{\infty}$ and $\{\omega_n\}_{n=1}^{\infty}$ with $\alpha_n \in \mathbf{R}$, $\omega_n > 0$, such that

$$P_0(x) = 1, P_1(x) = x - \alpha_1,$$
(5.10)

$$xP_n(x) = P_{n+1}(x) + \alpha_{n+1}P_n(x) + \omega_n P_{n-1}(x), \quad n = 1, 2, \dots$$
(5.11)

Moreover,

$$||P_0|| = 1, \quad ||P_n||^2 = \omega_1 \omega_2 \cdots \omega_n, \quad n \ge 1,$$
 (5.12)

$$\alpha_1 = M_1(\mu) = \text{mean}(\mu) = \int_{-\infty}^{+\infty} x\mu(dx),$$
(5.13)

$$\omega_1 = \operatorname{var}(\mu) = \int_{-\infty}^{+\infty} (x - \alpha_1)^2 \mu(dx).$$
 (5.14)

PROOF. Well known and omitted.

Definition 5.3.3 We call the pair of sequences $(\{\alpha_n\}_{n=1}^{\infty}, \{\omega_n\}_{n=1}^{\infty})$ the Jacobi coefficients.

Remark 5.3.4 Setting $P_{-1} = 0$ and understanding $\omega_0 P_{-1} = 0$, we regard (5.11) is valid also for n = 0. Remind that ω_0 is not defined.

Remark 5.3.5 If the orthogonal polynomials consists of m_0 polynomials, we understand the Jacobi coefficients are given by $(\{\alpha_1, \alpha_2, \ldots, \alpha_{m_0}\}, \{\omega_1, \omega_2, \ldots, \omega_{m_0-1}\})$.

5.4 States on Adjacency Algebras

Definition 5.4.1 Let \mathcal{A} be a *-algebra over \mathbf{C} with the multiplication unit $1_{\mathcal{A}}$. A function $\varphi : \mathcal{A} \to \mathbf{C}$ is called a *state* on \mathcal{A} if

(i) φ is linear;

(ii)
$$\varphi(a^*a) \ge 0$$
 for all $a \in \mathcal{A}$;

(iii) $\varphi(1_{\mathcal{A}}) = 1.$

We shall define two basic states on the adjacency algebra $\mathcal{A}(G)$ of a graph G.

(1) Assume that $|V| < \infty$. We define $\varphi_{tr} : \mathcal{A} \to \mathbf{C}$ by

$$\varphi_{\mathrm{tr}}(a) = \frac{1}{|V|} \mathrm{Tr}(a) = \frac{1}{|V|} \sum_{x \in V} (a)_{xx}, \qquad a \in \mathcal{A}(G).$$

One can check easily that φ_{tr} is a state on $\mathcal{A}(G)$. We call it the normalized trace.

(2) We fix $o \in V$. We define $\varphi_o : \mathcal{A} \to \mathbf{C}$ by

$$\varphi_o(a) = (a)_{oo}, \qquad a \in \mathcal{A}(G).$$

One can check easily that φ_o is a state on $\mathcal{A}(G)$. In fact, for positivity,

$$\varphi_o(a^*a) = (a^*a)_{oo} = \sum_{x \in V} (a^*)_{ox}(a)_{xo} = \sum_{x \in V} \overline{(a)_{xo}}(a)_{xo} \ge 0.$$

We call φ_o the vector trace at $o \in V$. In some contexts φ_o is also called the *vacuum state*.

Theorem 5.4.2 If G is a finite distance-regular graph, we have

 $\varphi_{\rm tr} = \varphi_o$ (as a state on the adjacency algebra $\mathcal{A}(G)$).

PROOF. Let $a \in \mathcal{A}(G)$. We see from Theorem 4.3.4 that a is a linear combination of distance matrices:

$$a = \sum_{k=0}^{d} c_k A^{(k)}.$$

Then, $(a)_{xx} = c_0$ for all $x \in V$, and $(a)_{xx} = (a)_{oo}$ Therefore,

$$\varphi_{\rm tr}(a) = \frac{1}{|V|} \sum_{x \in V} (a)_{xx} = (a)_{oo} = \varphi_o(a).$$

This proves the assertion.

5.5 Spectral Distribution of DRGs

We keep the notations and assumptions in Theorem 5.2.3. The main point is that, accroding to the quantum decomposition of the adjacency matrix $A = A^+ + A^- + A^\circ$, we found an interacting Fock space structure. Thus,

$$A\Phi_n = \sqrt{\omega_{n+1}} \Phi_{n+1} + \alpha_{n+1} \Phi_n + \sqrt{\omega_n} \Phi_{n-1}, \qquad n = 0, 1, 2, \dots,$$
(5.15)

where

$$\omega_n = b_{n-1}c_n, \qquad \alpha_n = a_{n-1}, \qquad n = 1, 2, \dots$$

5.5. SPECTRAL DISTRIBUTION OF DRGS

On the other hand, let μ be a probability measure on **R** with Jacobi coefficients ($\{\alpha_n\}, \{\omega_n\}$). (We shall prove later that such a probability measure exists and here let us assume this.) Then the associated orthogonal polynomials $\{P_n\}$ satisfies

$$xP_n(x) = P_{n+1}(x) + \alpha_{n+1}P_n(x) + \omega_n P_{n-1}(x) \,.$$

In view of $||P_n|| = \sqrt{\omega_n \cdots \omega_1}$ we have

$$x \frac{P_n(x)}{\sqrt{\omega_n \cdots \omega_1}} = \sqrt{\omega_{n+1}} \frac{P_{n+1}(x)}{\sqrt{\omega_{n+1} \cdots \omega_1}} + \alpha_{n+1} \frac{P_n(x)}{\sqrt{\omega_n \cdots \omega_1}} + \sqrt{\omega_n} \frac{P_{n-1}(x)}{\sqrt{\omega_{n-1} \cdots \omega_1}}.$$
 (5.16)

We define an isometry $U: \Gamma \to L^2(\mathbf{R}, \mu)$ by

$$U\Phi_n = \frac{P_n(x)}{\sqrt{\omega_n \cdots \omega_1}}, \qquad n = 0, 1, 2, \dots$$

Then, we have

$$(UAU^*f)(x) = xf(x), \qquad f \in L^2(\mathbf{R},\mu)$$

Since U is isometric,

$$\langle \Phi_0, A^m \Phi_0 \rangle = \langle U \Phi_0, U A^m \Phi_0 \rangle = \langle U \Phi_0, x^m U \Phi_0 \rangle$$

= $\langle P_0, x^m P_0 \rangle = \int_{-\infty}^{+\infty} x^m \mu(dx) = M_m(\mu)$

On the other hand, we have

$$\langle \Phi_0, A^m \Phi_0 \rangle = \langle e_o, A^m e_o \rangle = \varphi_o(A^m)$$

Consequently,

Theorem 5.5.1 Let G be a distance-regular graph with adjacency matrix A. Let $(\{\omega_n\}, \{\alpha_n\})$ be defined by

$$\omega_n = b_{n-1}c_n$$
, $\alpha_n = a_{n-1}$, $n = 1, 2, \dots$,

where a_n, b_n, c_n come from the intersection array of G. A probability measure μ satisfies

$$\varphi_o(A^m) = (A^m)_{oo} = M_m(\mu) = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots,$$

if and only if the Jacobi coefficients of μ coincide with $(\{\omega_n\}, \{\alpha_n\})$.

Theorem 5.5.2 Keeping the same notations as in Theorem 5.5.1, we assume in addition that G is a finite distance-regular graph. Then, the spectral distribution of G satisfies the conditions for μ .

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PROOF. Let ν be the spectral distribution of G. Then,

$$\varphi_{\rm tr}(A^m) = \int_{-\infty}^{+\infty} x^m \nu(dx), \qquad m = 1, 2, \dots,$$

On the other hand, we see from Theorem 5.4.2 that

$$\varphi_{\rm tr}(A^m) = \varphi_o(A^m).$$

Hence, we have

$$\int_{-\infty}^{+\infty} x^m \nu(dx) = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots$$

Since the Jacobi coefficients are determined through the Gram-Schmidt orthogonalization, they are uniquely determined by the moments. Hence the Jacobi coefficients of ν and μ coincide.

5.6 Exercises

(1) Find the Jacobi coefficients associated with the one-dimensional integer lattice \mathbb{Z} .

(2) Find the Jacobi coefficients associated with the homogeneous tree of degree κ . (\mathbb{Z} is the case of $\kappa = 2$)

Ans.
$$\omega_1 = \kappa, \, \omega_2 = \cdots = \kappa - 1, \quad \alpha_n \equiv 0.$$

(3) Prove that two probability measure $\mu, \nu \in \mathfrak{P}_{fm}(\mathbf{R})$ with the same moment sequences have the same Jacobi coefficients.

6 Adjacency Matrices as Algebraic Random Variables

6.1 Algebraic Probability Spaces

Definition 6.1.1 Let \mathcal{A} be a *-algebra over \mathbf{C} with multiplication unit $1_{\mathcal{A}}$. A function $\varphi : \mathcal{A} \to \mathbf{C}$ is called a *state* on \mathcal{A} is

- (i) φ is linear;
- (ii) $\varphi(a^*a) \ge 0;$
- (iii) $\varphi(1_{\mathcal{A}}) = 1.$

Then, the pair (\mathcal{A}, φ) is called an *algebraic probability space*.

Example 6.1.2 Let G = (V, E) be a locally finite graph and $\mathcal{A}(G)$ the adjacency algebra. Then,

$$\varphi_o(a) = (a)_{oo} = \langle e_o, ae_o \rangle, \qquad a \in \mathcal{A}(G),$$

where $e_o \in C(V)$ is defined by

$$e_o(x) = \begin{cases} 1, & \text{if } x = o, \\ 0, & \text{otherwise.} \end{cases}$$
(6.1)

Then $(\mathcal{A}(G), \varphi_o) = (\mathcal{A}(G), e_o)$ is an algebraic probability space. We sometimes call φ_o the vacuum state at $o \in V$.

Example 6.1.3 Let G = (V, E) be a finite graph with |V| = n. Define

$$\varphi_{\rm tr}(a) = \frac{1}{n} \sum_{x \in V} (a)_{xx} = \frac{1}{n} \sum_{x \in V} \langle e_x, ae_x \rangle, \qquad a \in \mathcal{A}(G),$$

where $e_x \in C(V)$ is defined as in (6.1). Then $(\mathcal{A}(G), \varphi_{tr})$ is an algebraic probability space. We call φ_{tr} the *normalized trace*.

Example 6.1.4 Let $\mathbf{C}[X]$ be the set of polynomials in the indeterminant X with complex coefficients. Equipped with the usual addition, scalar multiplication and product, $\mathbf{C}[X]$ becomes a commutative algebra. Moreover, we define the involution (*-operation) by

$$(c_0 + c_1 X + \dots + c_n X^n)^* = \overline{c_0} + \overline{c_1} X + \dots + \overline{c_n} X^n.$$

Thus, $\mathbf{C}[X]$ becomes a *-algebra. Let $\mathfrak{P}_{fm}(\mathbf{R})$ be the set of probability measures on \mathbf{R} that admit finite moments of all orders. Let $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$. Then

$$P \mapsto \int_{-\infty}^{+\infty} P(x)\mu(dx) \equiv \mu(P), \qquad P \in \mathbf{C}[X],$$

is a state on $\mathbb{C}[X]$. Thus, $(\mathbb{C}[X], \mu)$ is an algebraic probability space.

Example 6.1.5 Let $\{\omega_n\}$ be a Jacobi sequence and $(\Gamma, \{\Phi_n\}, B^+, B^-)$ be the associated interacting Fock space, i.e.,

$$B^{+}\Phi_{n} = \sqrt{\omega_{n+1}} \Phi_{n+1}, \quad n = 0, 1, \dots,$$

$$B^{-}\Phi_{0} = 0, \quad B^{-}\Phi_{n} = \sqrt{\omega_{n}} \Phi_{n-1}, \quad n = 1, 2, \dots.$$

Let $\{\alpha_1, \alpha_2, \dots\}$ be a real sequence and define

$$B^{\circ}\Phi_n = \alpha_{n+1}\Phi_n, \quad n = 0, 1, 2, \dots$$

Then, we have $(B^+)^* = B^-$, $(B^-)^* = B^+$, $(B^\circ)^* = B^\circ$. Let \mathcal{A} be the *-algebra generated by B^+, B^-, B° , i.e., the set of all (noncommutative) polynomials in B^+, B^-, B° . Then the function φ_0 defined by

$$\varphi_0(a) = \langle \Phi_0, a\Phi_0 \rangle, \qquad a \in \mathcal{A}$$

is a state on \mathcal{A} . We call $(\mathcal{A}, \varphi_0) = (\mathcal{A}, \Phi_0)$ an interacting Fock probability space with vacuum state.

6.2 Distributions of Algebraic Random Variables

Definition 6.2.1 Let (\mathcal{A}, φ) be an algebraic probability space. An element $a \in \mathcal{A}$ is called an *algebraic random variable* or a *random variable* for short. If $a = a^*$, we call it *real*.

Theorem 6.2.2 Let (\mathcal{A}, φ) be an algebraic probability space and let $a = a^* \in \mathcal{A}$ be a real random variable. Then, there exists a probability measure $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$ such that

$$\varphi(a^m) = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots.$$
 (6.2)

Definition 6.2.3 A probability measure μ satisfying (6.2) is called the *distribution* of a in φ . As discussed later, μ is not uniquely determined in general.

PROOF. Set $M_m = \varphi(a^m)$ and consider the Hanckel determinant:

$$\Delta_m = |H_m|, \qquad H_m = \begin{bmatrix} M_0 & M_1 & \cdots & M_m \\ M_1 & M_2 & \cdots & M_{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ M_m & M_{m+1} & \cdots & M_{2m} \end{bmatrix}.$$
 (6.3)

It follows from Hamburger's theorem (1920) that there exists a probability measure $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$ such that

$$M_m = \int_{-\infty}^{+\infty} x^m \mu(dx), \qquad m = 1, 2, \dots$$

if and only if

(M1) $\Delta_m > 0$ for all m; or

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(M2) there exists $m_0 \ge 1$ such that $\Delta_1 > 0, \ldots, \Delta_{m_0-1} > 0$ and $\Delta_{m_0} = \cdots = 0$. We shall check this condition for our Δ_m defined in (6.3). For

$$oldsymbol{u} = egin{bmatrix} u_0 \ dots \ u_m \end{bmatrix} \in \mathbf{C}^{m+1}$$

we have

$$\langle \boldsymbol{u}, H_m \boldsymbol{u} \rangle = \sum_{i,j=0}^m \overline{u_i} M_{ij} u_j = \sum_{i,j=0}^m \overline{u_i} u_j \varphi(a^{i+j})$$

= $\varphi\left(\sum_{i,j=0}^m \overline{u_i} u_j a^{i+j}\right) = \varphi\left(\left(\sum_{i=0}^m u_i a_i\right)^* \left(\sum_{j=0}^m u_j a^j\right)\right) \ge 0,$

which shows that H_m is positive definite. Hence its eigenvalues are all non-negative real numbers and $\Delta_m \geq 0$.

We next show that $\Delta_m = 0$ implies $\Delta_{m+1} = 0$. Suppose that $\Delta_m = 0$. Then there exists $\boldsymbol{u} \neq \boldsymbol{0}$ such that $H_m \boldsymbol{u} = \boldsymbol{0}$. Set

$$oldsymbol{v} = egin{bmatrix} oldsymbol{u} \ 0 \end{bmatrix} \in \mathbf{C}^{m+2}.$$

Apparently, $\boldsymbol{v} \neq \boldsymbol{0}$. Since

$$H_{m+1}\boldsymbol{v} = \begin{bmatrix} H_m & \ast \\ \ast & M_{2m} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ 0 \end{bmatrix} = \begin{bmatrix} H_m \boldsymbol{u} \\ \ast \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ \ast \end{bmatrix},$$

we have

$$\langle \boldsymbol{v}, H_{m+1}\boldsymbol{v} \rangle = 0.$$

Having shown that H_{m+1} is positive definite, we see that $\Delta_{m+1} = 0$.

6.3 The Moment Problem

Let \mathfrak{M} be the set of all real sequences $\{M_0 = 1, M_1, M_2, ...\}$ satisfying condition (M1) or (M2) in Section 6.2. It follows from Hamburger's theorem that the map $M : \mathfrak{P}_{fm}(\mathbf{R}) \to \mathfrak{M}$ defined by $M(\mu) = \{M_m(\mu)\}$ is surjective.

Definition 6.3.1 A probability measure $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$ is called the *solution of a determinate* moment problem if $M^{-1}(M(\mu)) = \{\mu\}$.

Proposition 6.3.2 (Carlemen's moment test) Let $\{M_m\} \in \mathfrak{M}$. If

$$\sum_{m=1}^{\infty} M_{2m}^{-\frac{1}{2m}} = +\infty,$$

then there exists a unique $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$ such that $M_m(\mu) = M_m$ for all $m = 1, 2, \ldots$

The proof is omitted, see e.g., Shohat–Tamarkin [11].

Example 6.3.3 (1) If supp (μ) is compact, then μ is the solution of a determinate moment problem.

(2) A classical Gaussian measure $N(m, \sigma^2)$ is the solution of a determinate moment problem. The density of the standard Gaussian measure N(0, 1) is given by

$$\frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

In fact, by the Stirling formula we have

$$M_{2m} = \frac{(2m)!}{2^m m!} \sim \sqrt{2} \left(\frac{2m}{e}\right)^m$$

(3) The classical Poisson measure with parameter $\lambda > 0$ is defined by

$$p_{\lambda} = e^{-\lambda} \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \, \delta_k \, .$$

The Poisson measure is the solution of a determinate moment problem. It is easily verified that $M_m \leq (\lambda + m)^m$.

Recall that, given $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$, we obtain a pair of sequences $(\{\omega_n\}, \{\alpha_n\})$, called the *Jacobi coefficients*, from the three-term recurrence relation (Theorem 5.3.2) satisfied by the orthogonal polynomials $\{P_n\}$ associated with μ . Let \mathfrak{J} be the set of pairs of sequences $(\{\omega_n\}, \{\alpha_n\})$ satisfying

- (i) for all $m, \omega_m > 0$ and $\alpha_1, \alpha_2, \ldots$ form an infinite sequence of real numbers; or
- (ii) there exists $m_0 \ge 1$ such that $\omega_1 > 0, \ldots, \omega_{m_0-1} > 0$ and $\omega_{m_0} = \omega_{m_0+1} = \cdots = 0$, and $\alpha_1, \alpha_2, \ldots, \alpha_{m_0}$ is a finite sequence of real numbers.

Since the Jacobi coefficients of a probability measure satisfy the above condition, we have a map

$$J: \mathfrak{P}_{\mathrm{fm}}(\mathbf{R}) \to \mathfrak{J}.$$

On the other hand, since the Gram-Schmidt orthogonalization is performed by using the moments of μ , the Jacobi coefficients ({ ω_n }, { α_n }) depend only on { $Mm(\mu)$ }. Therefore, the map $F : \mathfrak{M} \to \mathfrak{J}$ is defined by the commutative diagram:



Theorem 6.3.4 The map $F : \mathfrak{M} \to \mathfrak{J}$ is bijective.

The proof is omitted, see e.g., Hora–Obata [3].

Remark 6.3.5 $F^{-1}: \mathfrak{J} \to \mathfrak{M}$ is expressed explicitly by the Accardi–Bożejko formula [12].

Proposition 6.3.6 (Carleman) Let $\mu \in \mathfrak{P}_{fm}(\mathbf{R})$ and $(\{\omega_n\}, \{\alpha_n\})$ be its Jacobi coefficients. If

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt{\omega_n}} = +\infty,$$

then μ is the solution of a determinate moment problem. (If $\{\omega_n\}$ contains 0, we understand the above condition is satisfied.)

With the above argument, the spectral distributions in Theorems 5.5.1 and 5.5.2 are uniquely characterized by the Jacobi coefficients obtained from the intersection array of G.

6.4 Deformed Vacuum States

Definition 6.4.1 Let G = (V, E) be a connected graph. Given $q \in \mathbb{C}$, the matrix $Q = Q_q$ indexed by $V \times V$ defined by

$$(Q)_{xy} = q^{\partial(x,y)}, \qquad x, y \in V$$

is called the *Q*-matrix of *G*. For q = 0 we understand that $0^0 = 1$ and $Q_0 = E$ (the identity matrix).

The *Q*-matrix is related to the adjacency matrix: $\frac{d}{dq} Q\Big|_{q=0} = A.$



The Q-matrix gives rise to a one-parameter deformation of the vacuum state. Let us define

$$\langle a \rangle_q = \langle Q \delta_o, a \delta_o \rangle = \sum_{x \in V} q^{\partial(x,o)} \langle \delta_x, a \delta_o \rangle, \qquad a \in \mathcal{A}(G).$$
 (6.4)

Obviously, $\mathcal{A}(G) \ni a \mapsto \langle a \rangle_q$ is a normalized linear function on $\mathcal{A}(G)$. Being slightly free from the strict wording of "state," we give the following

Definition 6.4.3 A normalized linear function defined in (6.4) is called a *deformed vacuum* state on $\mathcal{A}(G)$.

Thus, a deformed vacuum state is not necessarily a state so conditions for its positivity are important to study. We recall the following general notion.

Definition 6.4.4 Let T be a matrix indexed by $V \times V$. We say that T is *positive definite* if

$$\langle f, Tf \rangle \ge 0$$
 for all $f \in C(V)$.

A positive definite matrix T is called *strictly positive definite* if

$$\langle f, Tf \rangle > 0$$
 for all $f \in C(V), f \neq 0$.

Proposition 6.4.5 The normalized linear function $\langle \cdot \rangle_q$ defined by (6.4) is positive, hence a state on $\mathcal{A}(G)$ if the following two conditions are fulfilled:

- (i) Q is a positive definite kernel on V;
- (ii) QA = AQ. (Note that Q is not necessarily locally finite but A is. Therefore the matrix elements of both sides are well-defined.)

PROOF. Let $a \in \mathcal{A}(G)$. Since a is a polynomial in A, we have Qa = aQ. Then, by the definition (6.4) we have

$$\langle a^*a \rangle_q = \langle Q\delta_o, a^*a\delta_o \rangle = \langle aQ\delta_o, a\delta_o \rangle = \langle Qa\delta_o, a\delta_o \rangle \ge 0,$$

which proves the assertion.

Proposition 6.4.6 Let $\mathcal{G} = (V, E)$ be a graph with $|V| \ge 2$. If $Q = (q^{\partial(x,y)})$ is a positive definite kernel on V, then $-1 \le q \le 1$.

PROOF. By assumption there is a pair of $a, b \in V$ such that $\partial(a, b) = 1$. Since $Q = (q^{\partial(x,y)})$ is a positive definite kernel on V, taking $f = \alpha \delta_a + \beta \delta_b$ in $C_0(V)$, we obtain

$$\left\langle \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \begin{bmatrix} 1 & q \\ q & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right\rangle \ge 0, \qquad \alpha, \beta \in \mathbf{C}, \tag{6.5}$$

where $\langle \cdot, \cdot \rangle$ is the usual Hermitian inner product of \mathbb{C}^2 . Therefore, the 2×2 matrix appearing in (6.5) is positive definite. Hence $q \in \mathbb{R}$ and $1 - q^2 \ge 0$.

Thus, the main question, which is quite open, is to determine the range of $q \in [-1, 1]$ for which Q becomes positive definite. See Bożejko [13] for the case of the star product of graphs.

In order to derive a sufficient condition for the equality QA = AQ we consider a geometric property of a graph. A graph G = (V, E) is called *quasi-distance-regular* if

$$\left| \left\{ z \in V \, ; \begin{array}{l} \partial(z,x) = n \\ \partial(z,y) = 1 \end{array} \right\} \right| = \left| \left\{ z \in V \, ; \begin{array}{l} \partial(z,x) = 1 \\ \partial(z,y) = n \end{array} \right\} \right| \tag{6.6}$$

holds for any choice of $x, y \in V$ and $n = 0, 1, 2, \ldots$ Here the number defined by (6.6) may depend on the choice of $x, y \in V$.

By definition, a distance-regular graph is quasi-distance-regular. On the other hand, if (6.6) depends only on $\partial(x, y)$, the graph G becomes distance-regular.

6.5. EXERCISES

Proposition 6.4.7 If a graph is quasi-distance-regular, then QA = AQ for all $q \in \mathbf{R}$. Conversely, if QA = AQ holds for q running over a non-empty open interval, then the graph is quasi-distance-regular.

PROOF. Let $x, y \in V$. Then

$$(QA)_{xy} = \sum_{z \in V} q^{\partial(x,z)} A_{zy} = \sum_{z \sim y} q^{\partial(x,z)}$$

= $\sum_{n=0}^{\infty} q^n |\{z \in V; \ \partial(z,x) = n, \ \partial(z,y) = 1\}|,$ (6.7)

which is in fact a finite sum. Similarly, we have

$$(AQ)_{xy} = \sum_{n=0}^{\infty} q^n |\{z \in V; \, \partial(z, x) = 1, \, \partial(z, y) = n\}|.$$
(6.8)

Hence, if the graph is quasi-distance-regular, the coefficients of q^n in (6.7) and (6.8) coincide and we obtain $(QA)_{xy} = (AQ)_{xy}$ for all $x, y \in V$. The converse assertion is readily clear.

6.5 Exercises

(1) Verify the statements in Example 6.3.3.

(2) Determine the range of q for which the Q-matrix of Example 6.4.2 (2) is positive deinite.

(3) Determine the range of q for which the Q-matrix of an octahedron is positive definite.



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Ans. $-2 + \sqrt{3} \le q \le 1$

7 Hamming Graphs

7.1 Definition and Some Properties

Let F be a finite set with $|F| = N \ge 2$, say $F = \{1, 2, ..., N\}$, and consider the cartesian product of $d \ge 1$ copies of F:

$$F^{d} = \{ x = (\xi_{1}, \dots, \xi_{d}) ; \xi_{i} \in F, \ 1 \le i \le d \}.$$

For $x = (\xi_1, \ldots, \xi_d), y = (\eta_1, \ldots, \eta_d) \in F^d$ define

$$\partial(x, y) = |\{1 \le i \le d ; \xi_i \ne \eta_i\}|.$$

Then ∂ becomes a distance function on F^d , which is called the *Hamming distance*.

Definition 7.1.1 The pair

$$V = F^d, \qquad E = \{\{x, y\} \, ; \, x, y \in F^d, \, \partial(x, y) = 1\}$$

is called a Hamming graph and is denoted by H(d, N).

We avoid the trivial case of N = 1 since H(d, 1) is a trivial graph, i.e., consists of a single vertex. H(d, 2) is the *d*-cube and H(2, N) is the $N \times N$ -grid. Furthermore, $H(1, N) \cong K_N$ (the complete graph with N vertices).



Figure 7.1: Hamming graphs H(2, 2), H(3, 2) and H(4, 2)

Remark 7.1.2 The graph distance of a Hamming graph $H(d, N) = (F^d, E)$ coincides with the Hamming distance on F^d .

Proposition 7.1.3 A Hamming graph H(d, N) is distance-transitive, hence distance-regular.

PROOF. A Hamming graph is highly symmetric. Let S(d) denote the symmetric group of degree d, i.e. the group of permutations of $\{1, 2, \ldots, d\}$, which acts on $H(d, N) = (F^d, E)$ by coordinate permutation:

$$\sigma x = (\xi_{\sigma^{-1}(1)}, \dots, \xi_{\sigma^{-1}(d)}), \quad \sigma \in S(d).$$

On the other hand, the direct product group $S(N)^d$ acts on H(d, N) by

$$\tau x = (\tau_1(\xi_1), \dots, \tau_d(\xi_d)), \quad \tau = (\tau_1, \dots, \tau_d) \in S(N)^d$$

Both actions give rise to automorphisms of H(d, N). By a simple observation we have

 $\sigma^{-1}\tau\sigma x = (\tau_{\sigma(1)}(\xi_1), \dots, \tau_{\sigma(d)}(\xi_d)) = \tau^{\sigma} x,$

where

$$\tau^{\sigma} = (\tau_1, \ldots, \tau_d)^{\sigma} = (\tau_{\sigma(1)}, \ldots, \tau_{\sigma(d)}).$$

Thus, the actions of S(d) and $S(N)^d$ generate a semidirect product group $S(d) \ltimes S(N)^d$. The assertion is proved with the help of the group action.

Remark 7.1.4 The action of $S(d) \ltimes S(N)^d$ on H(d, N) is transitive and the isotropy group of a vertex $o = (N, N, \dots, N)$ is $S(d) \ltimes S(N-1)^d$. Hence

$$H(d, N) \cong S(d) \ltimes S(N)^d / S(d) \ltimes S(N-1)^d.$$

In fact, it is shown that $\operatorname{Aut}(H(d, N)) \cong S(d) \ltimes S(N)^d$.

Proposition 7.1.5 diam H(d, N) = d and the degree is $\kappa_{d,N} = d(N-1)$.

Proposition 7.1.6 The intersection array of the Hamming graph H(d, N) is given with

$$a_n = p_{1n}^n = n(N-2), \quad b_n = p_{1,n+1}^n = (d-n)(N-1), \quad c_n = p_{1,n-1}^n = n,$$
 (7.1)

for $n = 0, 1, 2, \ldots, d$.

PROOF. We prove the first identity. Take two vertices $x, y \in V$ with $\partial(x, y) = n$. Without loss of generality we may set

$$x = (\underbrace{1, \dots, 1}_{n}, 1, \dots, 1), \qquad y = (\underbrace{2, \dots, 2}_{n}, 1, \dots, 1)$$

A vertex $z \in V$ with $\partial(x, z) = 1$ is of the form

$$z = (1, \ldots, i, \ldots, 1),$$

where $i \neq 1$ occurs at an arbitrary position. Among such z we need to determine ones with $\partial(y, z) = n$. Consider first the case where *i* occurs in the first *n* positions. Then, comparing

$$z = (1, \dots, i, \dots, 1, 1, \dots, 1),$$

 $y = (\underbrace{2, \dots, 2, \dots, 2}_{n}, 1, \dots, 1),$

we see that $\partial(y, z) = n$ if $i \neq 2$. Since such an *i* is chosen from $\{3, 4, \ldots, N\}$ and there are *n* positions, the number of *y* satisfying the above conditions is n(N-2). Next we consider the case where *i* occurs in the last d - n positions. Then we have

$$z = (1, \dots, 1, 1, \dots, i, \dots, 1),$$

$$y = (\underbrace{2, \dots, 2}_{n}, 1, \dots, 1, \dots, 1),$$

so that $\partial(y, z) = n + 1$, which does not satisfy the requirement $\partial(y, z) = n$. Consequently, $a_n = p_{1n}^n = n(N-2)$. The rest of (7.1) is shown easily in a similar fashion.

7.2 Spectral Analysis

7.2.1 Spectral Distributions in the Vacuum States

Theorem 7.2.1 Let $\mu_{d,N}$ be the spectral distribution of H(d, N) in the vacuum state. Then $\mu_{d,N}$ is uniquely specified the Jacobicoefficients given by

$$\omega_n = n(d - n + 1)(N - 1), \qquad n = 1, 2, \dots, d,$$

$$\alpha_n = (n - 1)(N - 2), \qquad n = 1, 2, \dots, d, d + 1.$$

PROOF. By combining Theorem 5.5.2 and Proposition 7.1.6.

Fixing $o \in V$ as an origin, consider the quantum decomposition:

$$A = A^+ + A^- + A^\circ.$$

Then, Theorem 7.2.1 says that

$$A^{+}\Phi_{n} = \sqrt{\omega_{n+1}} \Phi_{n+1} = \sqrt{(n+1)(d-n)(N-1)} \Phi_{n+1}, \qquad (7.2)$$

$$A^{-}\Phi_{n} = \sqrt{\omega_{n}} \Phi_{n-1} = \sqrt{n(d-n+1)(N-1)} \Phi_{n-1}, \qquad (7.3)$$

$$A^{\circ}\Phi_n = \alpha_{n+1}\Phi_n = n(N-2)\Phi_n.$$
(7.4)

7.2.2 Asymptotic Spectral Distributions in the Vacuum State

Consider growing Hamming graphs H(d, N) as $d \to \infty$ and $N \to \infty$. In view of (7.2)–(7.4), the coefficients of actions of A^{ϵ} diverges as $d \to \infty$ and $N \to \infty$. We need normalization to obtain a reasonable limit.

Note first that

$$\varphi_{\mathrm{tr}}(A) = \varphi_o(A) = 0, \qquad \varphi_{\mathrm{tr}}(A^2) = \varphi_o(A^2) = \mathrm{deg}(o) = \kappa_{d,N} = d(N-1).$$

Therefore, the variance of A diverges as $d \to \infty$ and $N \to \infty$. A reasonable normalization is

$$\frac{A}{\sqrt{d(N-1)}} \, .$$

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Thus, for (7.2)–(7.4) we consider

$$\frac{A^+}{\sqrt{d(N-1)}} \Phi_n = \sqrt{(n+1)\left(1-\frac{n}{d}\right)} \Phi_{n+1}, \qquad (7.5)$$

$$\frac{A^{-}}{\sqrt{d(N-1)}} \Phi_n = \sqrt{n\left(1 - \frac{n-1}{d}\right)} \Phi_{n-1}, \qquad (7.6)$$

$$\frac{A^{\circ}}{\sqrt{d(N-1)}} \Phi_n = n \sqrt{\frac{N-2}{d}} \sqrt{\frac{N-2}{N-1}} \Phi_n \,.$$
(7.7)

We observe that the coefficients on the right-hand sides converge as $d \to \infty$, $N \to \infty$, and

$$\frac{N}{d} \to \tau, \qquad \tau \in [0, +\infty).$$

In fact, the actions in this limit would be

$$\lim \frac{A^+}{\sqrt{d(N-1)}} \Phi_n = \sqrt{n+1} \Phi_{n+1},$$
$$\lim \frac{A^-}{\sqrt{d(N-1)}} \Phi_n = \sqrt{n} \Phi_{n-1},$$
$$\lim \frac{A^\circ}{\sqrt{d(N-1)}} \Phi_n = n\sqrt{\tau} \Phi_n.$$

However, the vectors Φ_n also depending on d, N, the limit does not make sense in this form.

For the actions appearing in the limit are described in terms of Boson Fock space. Let $(\Gamma = \Gamma_{\text{Boson}}, \{\Psi_n\}, B^+, B^-)$ be the Boson Fock space, where

$$B^{+}\Psi_{n} = \sqrt{n+1}\Psi_{n+1}, \qquad n = 0, 1, 2, \dots,$$

$$B^{-}\Psi_{0} = 0, \quad B^{-}\Psi_{n} = \sqrt{n}\Phi_{n-1}, \qquad n = 1, 2, \dots$$

Theorem 7.2.2 (QCLT for Hamming graphs) For any choice of $\epsilon_1, \ldots, \epsilon_m \in \{+, -, \circ\}$, $m = 1, 2, \ldots$, we have

$$\lim_{\substack{N/d \to \tau \\ d, N \to \infty}} \left\langle \Phi_0, \frac{A_{d,N}^{\epsilon_m}}{\sqrt{\kappa_{d,N}}} \cdots \frac{A_{d,N}^{\epsilon_1}}{\sqrt{\kappa_{d,N}}} \Phi_0 \right\rangle = \langle \Psi_0, B^{\epsilon_m} \cdots B^{\epsilon_1} \Psi_0 \rangle.$$
(7.8)

In short,

$$\lim_{\substack{N/d \to \tau \\ d, N \to \infty}} \frac{A_{d,N}^{\epsilon}}{\sqrt{\kappa_{d,N}}} = B^{\epsilon}, \qquad \epsilon \in \{+, -, \circ\},$$
(7.9)

in the sense of stochastic convergence with respect to the vacuum states.

PROOF. First we note that, for any $k, l \in \{0, 1, 2, ...\}$ and $\epsilon \in \{+, -, \circ\}$,

$$\lim_{\substack{N/d \to \tau \\ d, N \to \infty}} \left\langle \Phi_k, \frac{A_{d,N}^{\epsilon}}{\sqrt{\kappa_{d,N}}} \Phi_l \right\rangle = \langle \Psi_k, B^{\epsilon} \Psi_l \rangle.$$

Then, the result follows by induction.

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Theorem 7.2.3 (CLT for Hamming graphs) For m = 1, 2, ... we have

$$\lim_{\substack{N/d \to \tau \\ d,N \to \infty}} \left\langle \Phi_0, \left(\frac{A_{d,N}}{\sqrt{\kappa_{d,N}}}\right)^m \Phi_0 \right\rangle = \langle \Psi_0, (B^+ + B^- + \sqrt{\tau} B^+ B^-)^m \Psi_0 \rangle.$$
(7.10)

PROOF. We note that

$$\frac{A_{d,N}}{\sqrt{\kappa_{d,N}}} = \frac{A_{d,N}^+}{\sqrt{\kappa_{d,N}}} + \frac{A_{d,N}^-}{\sqrt{\kappa_{d,N}}} + \frac{A_{d,N}^\circ}{\sqrt{\kappa_{d,N}}} \to B^+ + B^- + B^\circ,$$

where

$$B^{\circ}\Phi_n = n\sqrt{\tau}\,\Phi_n.$$

On the other hand, by definition we have

 $B^+B^-\Phi_n = n\Phi_n,$

so that

$$B^{\circ} = \sqrt{\tau} B^+ B^-.$$

Thus, (7.10) is a consequence of (7.8).

7.2.3 Boson Fock Space

The most fundamental object is $B^+ + B^-$, which is sometimes referred to as the field operator.

Lemma 7.2.4 The vacuum spectral distribution of $B^+ + B^-$ is the standard Gaussian measure, *i.e.*,

$$\langle \Psi_0, (B^+ + B^-)^m \Psi_0 \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} x^m e^{-x^2/2} dx, \qquad m = 1, 2, \dots$$

PROOF. Well known.

Another interesting operator is the number operator $N = B^+B^-$, which acts as

$$B^+B^-\Psi_n = n\Psi_n, \qquad n = 0, 1, 2, \dots$$

Lemma 7.2.5 For $\lambda > 0$, the vacuum spectral distribution of $(B^+ + \sqrt{\lambda})(B^- + \sqrt{\lambda})$ is the Poisson distribution with parameter λ , denoted by p_{λ} , see Example 6.3.3. In other words,

$$\langle \Psi_0, ((B^+ + \sqrt{\lambda})(B^- + \sqrt{\lambda}))^m \Psi_0 \rangle = \int_{-\infty}^{+\infty} x^m p_\lambda(dx), \quad m = 1, 2, \dots$$
(7.11)

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PROOF. For simplicity we set

$$C^{+} = B^{+} + \sqrt{\lambda}, \quad C^{-} = B^{-} + \sqrt{\lambda}.$$

Since $B^{-}B^{+} = B^{+}B^{-} + 1$, we have

$$C^{-}C^{+} = B^{-}B^{+} + \sqrt{\lambda} (B^{+} + B^{-}) + \lambda = C^{+}C^{-} + 1.$$

Hence for $m = 1, 2, \ldots$ we have

$$(C^{+}C^{-})^{m} = C^{+}(C^{-}C^{+})^{m-1}C^{-} = C^{+}(C^{+}C^{-}+1)^{m-1}C^{-}.$$
(7.12)

Let M_m denote the left-hand side of (7.11), namely, the moment sequence of the algebraic random variable C^+C^- in the vacuum state:

$$M_m = \langle \Phi_0, (C^+C^-)^m \Psi_0 \rangle, \qquad m = 1, 2, \dots$$

Then, by (7.12) and the obvious identity $C^{-}\Psi_{0} = \sqrt{\lambda} \Psi_{0}$, we come to

$$M_m = \langle C^- \Psi_0, (C^+ C^- + 1)^{m-1} C^- \Psi_0 \rangle = \lambda \langle \Psi_0, (C^+ C^- + 1)^{m-1} \Psi_0 \rangle.$$

By the binomial expansion the last expression becomes

$$M_m = \lambda \sum_{k=0}^{m-1} {m-1 \choose k} M_k, \quad m = 1, 2, \dots$$

It is obvious that $M_0 = 1$.

On the other hand, as we see directly from the definition, the moment sequence of the Poisson measure with parameter λ satisfies the same recurrence relation for M_m . Hence (7.11) follows.

7.2.4 Asymptotic Spectral Distributions of H(d, m) in the Limit

We are now in a position to describe the limit measure

$$\lim_{\substack{N/d \to \tau \\ d, N \to \infty}} \mu_{d, N}$$

where $\mu_{d,N}$ is the spectral distribution of the Hamming graph H(d, N). By Theorem 7.2.3 we have

$$\lim_{\substack{N/d \to \tau \\ d, N \to \infty}} \int_{-\infty}^{+\infty} \left(\frac{x}{\sqrt{d(N-1)}} \right)^m \mu_{d,N}(dx) = \langle \Psi_0, (B^+ + B^- + \sqrt{\tau} B^+ B^-)^m \Psi_0 \rangle.$$
(7.13)

We start with the case of $\tau = 0$. Applying Lemma 7.2.4, we see that

$$\lim_{\substack{N/d \to 0 \\ d, N \to \infty}} \int_{-\infty}^{+\infty} \left(\frac{x}{\sqrt{d(N-1)}}\right)^m \mu_{d,N}(dx) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} x^m e^{-x^2/2} dx, \qquad m = 1, 2, \dots.$$

This means that the normalized spectral distribution of the Hamming graph H(d, N) converges to the standard Gaussian measure in the sense of moments. Since the standard Gaussian measure is the solution of a determinate moment problem, by a general result we may conclude the weak convergence too. Summing up,

Theorem 7.2.6 The normalized spectral distribution of the Hamming graph H(d, N) converges in the limit as $d, N \to \infty$, $N/d \to 0$, to the standard Gaussian measure in the sense of moments and weak convergence of probability measures.

We next consider the case of $\tau > 0$. Note that

$$B^{+} + B^{-} + \sqrt{\tau} B^{+} B^{-} = \sqrt{\tau} \left(B^{+} + \frac{1}{\sqrt{\tau}} \right) \left(B^{-} + \frac{1}{\sqrt{\tau}} \right) - \frac{1}{\sqrt{\tau}}$$

and the distribution of $\left(B^+ + \frac{1}{\sqrt{\tau}}\right)\left(B^- + \frac{1}{\sqrt{\tau}}\right)$ is the classical Poisson measure with parameter $1/\sqrt{\tau}$ by Lemma 7.2.5. Thus, the limit of the normalized spectral distribution of the Hamming graph H(d, N) is a simple affine transformation (dilation and translation) of the clasical Posson measure. In fact, we conclude that

Theorem 7.2.7 The normalized spectral distribution of the Hamming graph H(d, N) converges in the limit as $d, N \to \infty$, $N/d \to \tau > 0$, to ν_{τ} in the sense of moments and weak convergence of probability measures. Here ν_{τ} is an affine transformation of the classical Poisson measure with parameter $1/\sqrt{\tau}$, given by

$$\nu_{\tau} = e^{-1/\tau} \sum_{k=0}^{\infty} \frac{\tau^{-k}}{k!} \,\delta_{k\sqrt{\tau} - \frac{1}{\sqrt{\tau}}}$$

Remark 7.2.8 The Hamming graph H(d, N) is the direct product of d copies of the complete graph K_N . This fact gives another aspect to the asymptotic spectral analysis and will be discussed later.

7.3 Exercises

(1) Show that the graph distance of a Hamming graph $H(d, N) = (F^d, E)$ coincides with the Hamming distance on F^d .

(2) Let $\Gamma_{\text{Boson}} = (\Gamma, \{\Psi_n\}, B^+, B^-)$ be the Boson Fock space and set

$$B^{\circ} = \frac{1}{\sqrt{\lambda}} B^{+} B^{-} + \sqrt{\lambda}.$$

Using the identity

$$\langle \Psi_0, (B^+ + B^- + B^\circ)^m \Psi_0 \rangle = \int_{-\infty}^{+\infty} \left(\frac{x}{\sqrt{\lambda}}\right)^m p_\lambda(dx), \quad m = 1, 2, \dots,$$

show that the Jacobi coefficients $(\{\omega_n\}, \{\alpha_n\})$ of the Poisson distribution with parameter $\lambda > 0$ is given by

$$\omega_n = \lambda n, \quad \alpha_n = n - 1 + \lambda, \qquad n = 1, 2, \dots$$