STUDIA MATHEMATICA 179 (1) (2007)

Positive Q-matrices of graphs

by

Nobuaki Obata (Sendai)

Abstract. The Q-matrix of a connected graph $\mathcal{G} = (V, E)$ is $Q = (q^{\partial(x,y)})_{x,y\in V}$, where $\partial(x, y)$ is the graph distance. Let $q(\mathcal{G})$ be the range of $q \in (-1, 1)$ for which the Q-matrix is strictly positive. We obtain a sufficient condition for the equality $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$ where $\widetilde{\mathcal{G}}$ is an extension of a finite graph $\mathcal{G}$ by joining a square. Some concrete examples are discussed.

1. Introduction. Associated with a graph, various matrices have been introduced and studied extensively, e.g., adjacency matrix, distance matrix, graph Laplacian, transition matrix and so forth. Applications of these matrices spread widely from discrete mathematics to analysis and geometry; see, e.g., Biggs [1], Cvetković–Doob–Sachs [6], Simon [14] and references cited therein. Our concern in this paper is positivity of the Q-matrix of a graph, which is an important question in harmonic analysis.

Let $\mathcal{G} = (V, E)$ be a connected graph and $\partial(x, y)$ the graph distance. The *Q-matrix* of $\mathcal{G}$ is defined by

$$Q = Q_q = (q^{\partial(x,y)})_{x,y\in V}, \qquad q \in \mathbb{C}. \tag{1.1}$$

Let $\widetilde{q}(\mathcal{G})$ denote the set of $q \in \mathbb{C}$ for which Q_q is positive. It is known that $\widetilde{q}(\mathcal{G}) \subset [-1, 1]$ unless $\mathcal{G}$ is trivial, i.e., consists of a single vertex. Let $q(\mathcal{G}) \subset \widetilde{q}(\mathcal{G})$ denote the set of $q \in \mathbb{C}$ for which Q_q is strictly positive. It is an important problem in harmonic analysis to determine $q(\mathcal{G})$ and $\widetilde{q}(\mathcal{G})$. For example, the Q-matrix of a tree defines the so-called Haagerup state [9] and plays an essential role in harmonic analysis on free groups and related structures; see, e.g., Bożejko [2], Bożejko–Januszkiewicz–Spatzier [4], Bożejko–Szwarc [5], Figà-Talamanca–Picardello [8]. More recently, asymptotic spectral analysis of growing graphs have been intensively studied, where interesting states are defined by positive Q-matrices (see Hora–Obata [11, 12]).

However, it is difficult to determine $q(\mathcal{G})$ and $\widetilde{q}(\mathcal{G})$ in general. So far

2000 *Mathematics Subject Classification*: Primary 05C50; Secondary 43A35.
Key words and phrases: Q-matrix, graph, positive definite kernel, Markov sum.

two approaches have been proposed by Bożejko. The first one is known as the quadratic embedding test. Verifying a particular embedding of a graph into a Hilbert space (called a quadratic embedding), one concludes that Q_q is positive for all $0 \le q \le 1$. For example, Hamming graphs and Johnson graphs have this property (see, e.g., Hora [10]). The property of admitting a quadratic embedding seems to be rather strong, in fact, there are many small graphs which do not have this property or for which $[0,1] \subset \widetilde{q}(\mathcal{G})$ does not hold. Moreover, the quadratic embedding test brings no information about negative $q < 0$.

The second approach is more general and elegant. Bożejko [3] introduced a particular join of two positive definite matrices, called Markov sum, which is irrelevant to graph structure and covers many problems in harmonic analysis. Specializing his general result to the Q-matrices of graphs, one obtains immediately the following

Theorem 1.1 (Star product). *If $\widetilde{\mathcal{G}}$ is a star product of two graphs $\mathcal{G}$ and $\mathcal{G}_1$, then $q(\widetilde{\mathcal{G}}) = q(\mathcal{G}) \cap q(\mathcal{G}_1)$. If moreover $q(\mathcal{G}_1) = (-1,1)$, we have $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$.*

Here the *star product* is obtained by gluing two graphs at one common vertex. Since $q(C^2) = (-1,1)$, where C^2 is a graph with two vertices and one edge, we see that the Q-matrix of a tree is strictly positive for all $-1 < q < 1$. Thus the famous Haagerup theorem [9] is recovered. For the star product, see also Obata [13].

The aim of this paper is to obtain another extension of graphs which preserves the positivity of the Q-matrix. The essence of the star product is to join two graphs at a *single* common vertex. If two or more vertices are taken to join two graphs, the situation becomes fairly complicated. It seems, therefore, reasonable to start from extending a graph $\mathcal{G} = (V,E)$ by joining a square C^4. We consider three cases shown in Figure 1:

Case 1: *One-vertex detour extension making a square.* Taking $a, b \in V$

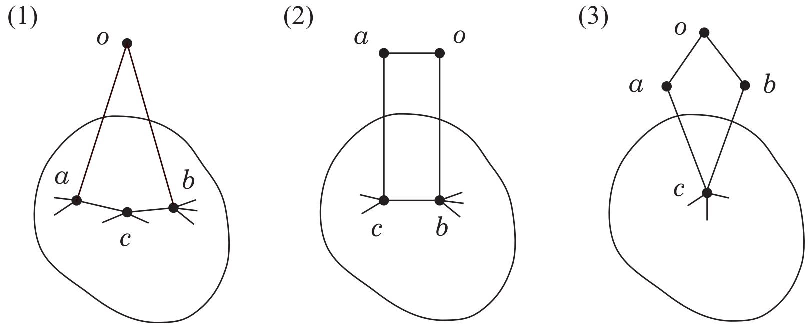

Fig. 1. Joining a square

with $\partial(a,b)=2$ and a new vertex o, we define a graph $\widetilde{\mathcal{G}}=(\widetilde{V},\widetilde{E})$ by

$$\widetilde{V}=V\cup\{o\},\qquad \widetilde{E}=E\cup\{\{o,a\},\{o,b\}\}.$$

In this case, $q(\widetilde{\mathcal{G}})=q(\mathcal{G})$ does not hold in general, so that we need an additional condition for the equality. We call $\widetilde{\mathcal{G}}$ an *admissible one-vertex detour extension making a square* if it satisfies the condition (H) described in Section 5.1.

CASE 2: *Square-concatenation.* Taking $b,c\in V$ with $\partial(b,c)=1$ and new vertices o,a, we define a graph $\widetilde{\mathcal{G}}=(\widetilde{V},\widetilde{E})$ by

$$\widetilde{V}=V\cup\{o,a\},\qquad \widetilde{E}=E\cup\{\{o,a\},\{o,b\},\{a,c\}\}.$$

CASE 3: *Star product with a square.* Taking $c\in V$ and new vertices o,a,b, we define a graph $\widetilde{\mathcal{G}}=(\widetilde{V},\widetilde{E})$ by

$$\widetilde{V}=V\cup\{o,a,b\},\qquad \widetilde{E}=E\cup\{\{o,a\},\{o,b\},\{a,c\},\{b,c\}\}.$$

MAIN THEOREM. *Let $\widetilde{\mathcal{G}}$ be a graph obtained from a finite graph $\mathcal{G}$ by joining a square. Then $q(\widetilde{\mathcal{G}})=q(\mathcal{G})$ if $\widetilde{\mathcal{G}}$ is* (i) *an admissible one-vertex detour extension making a square*; *or* (ii) *a square-concatenation*; *or* (iii) *a star product with a square.*

In the above assertion, the first two cases are essentially new, while case (iii) is a direct consequence of Theorem 1.1 combined with $q(C^4)=(-1,1)$.

This paper is organized as follows: Section 2 assembles some preliminary notions and facts. In Section 3 we define the Q-matrix and list some elementary properties. In Section 4 we introduce the notion of a detour join of two graphs and derive a general criterion for positivity of the Q-matrix. In Section 5, our main result is proved (Theorems 5.4 and 5.5). Section 6 contains some concrete examples.

2. Preliminaries. In order to avoid unnecessary confusion we assemble some basic notions and notations used throughout this paper. The facts mentioned here are standard.

Let V be a finite or infinite, non-empty set. Let $C_0(V)$ be the space of $\mathbb{C}$-valued functions defined on V with finite supports. When V is a finite set, we often write $C(V)$ for $C_0(V)$. Define an inner product on $C_0(V)$ by

$$\langle f,g\rangle=\sum_{x\in V}\overline{f(x)}\,g(x),\qquad f,g\in C_0(V).$$

By convention the notation $\langle f,g\rangle$ is used whenever the right hand side converges absolutely. Let T be a matrix with index set V, that is, T is a $\mathbb{C}$-valued function defined on $V\times V$. We often write $T=(T(x,y))_{x,y\in V}$. We say that a matrix $T = (T(x, y))$ is *positive* if

$$\langle f, Tf \rangle = \sum_{x,y \in V} \overline{f(x)}\, T(x, y) f(y) \geq 0 \quad \text{for all } f \in C_0(V).$$

PROPOSITION 2.1. *A positive matrix* $T = (T(x, y))$ *is hermitian symmetric, i.e.,* $T = T^*$, *or equivalently,* $T(x, y) = \overline{T(y, x)}$ *for all* $x, y \in V$.

REMARK 2.2. We shall be concerned mostly with real symmetric matrices. It is easy to see that a real symmetric matrix $T = (T(x, y))$ is positive if and only if

$$\langle f, Tf \rangle = \sum_{x,y \in V} f(x) T(x, y) f(y) \geq 0 \quad \text{for all } \textit{real } f \in C_0(V).$$

Let T be a matrix with index set V. For a non-empty subset $U \subset V$ the restriction of T to $U \times U$ is called a *principal submatrix* of T, and is denoted by $T \restriction U$. By definition, T is positive if and only if so is $T \restriction U$ for every finite subset $U \subset V$.

PROPOSITION 2.3. *T is positive if and only if for any finite subset $U \subset V$, every eigenvalue of $T \restriction U$ is non-negative.*

For a finite subset $U \subset V$, the determinant of $T \restriction U$ is defined, which is called a *principal minor* of T.

PROPOSITION 2.4. *T is positive if and only if every principal minor is non-negative, that is,* $\det T \restriction U \geq 0$ *for every finite subset* $U \subset V$.

We say that T is *strictly positive* if

$$\langle f, Tf \rangle > 0 \quad \text{for all } f \in C_0(V) \text{ with } f \neq 0.$$

When T is real and symmetric, the above condition can be replaced with "for all *real* $f \in C_0(V)$ with $f \neq 0$." Propositions 2.3 and 2.4 remain valid for strict positivity.

PROPOSITION 2.5. *T is strictly positive if and only if for any finite subset $U \subset V$, every eigenvalue of $T \restriction U$ is positive; moreover, if and only if* $\det T \restriction U > 0$ *for every finite subset* $U \subset V$.

When V is finite, we have the following stronger assertion.

PROPOSITION 2.6. *Let T be a matrix with a finite index set V, say $|V| = n$. If there exists an increasing sequence of subsets $U_1 \subset \cdots \subset U_n = V$ such that $|U_s| = s$ and* $\det T \restriction U_s > 0$ *for all $s = 1, \dots, n$, then T is strictly positive.*

As is well known, Proposition 2.6 does not remain valid for positivity, i.e., T is not necessarily positive even if $\det T \restriction U_s \geq 0$ for all $s = 1, \dots, n$.

3. The Q-matrix. A *graph* is a pair $\mathcal{G} = (V, E)$, where V is a non-empty (finite or infinite) set and E a subset of $\{\{x, y\}\,;\, x, y \in V,\ x \neq y\}$. Elements of V and E are called *vertices* and *edges*, respectively. If $\{x, y\} \in E$, we say that x and y are *adjacent* and write $x \sim y$ for simplicity. A finite sequence of vertices $x_0, x_1, \ldots, x_n$ is called a *walk* of length n if $x_0 \sim x_1 \sim \cdots \sim x_n$. If $x_0, x_1, \ldots, x_n$ are mutually distinct, the walk is called a *path* of length n. A graph is called *connected* if any pair of vertices are connected by a walk. Throughout the paper a graph is always assumed to be connected.

For $x, y \in V$ with $x \neq y$ let $\partial(x, y)$ denote the length of the shortest path connecting x and y. By definition we set $\partial(x, x) = 0$. Then $\partial(x, y)$ becomes a metric on V, which we call the *graph distance*.

Definition 3.1. Let $\mathcal{G} = (V, E)$ be a graph (always assumed to be connected) with graph distance $\partial(x, y)$. The *Q-matrix* of $\mathcal{G}$ is defined by

$$Q = Q_q = (q^{\partial(x,y)})_{x,y \in V}, \qquad q \in \mathbb{C}.$$

The derivatives Q_0' and Q_1' are the adjacency matrix and the distance matrix, respectively. Our main interest is to determine the range of q such that the Q-matrix is positive or strictly positive. Let $q(\mathcal{G})$ be the set of $q \in \mathbb{C}$ for which $Q = Q_q$ is strictly positive, and $\widetilde{q}(\mathcal{G})$ the set of $q \in \mathbb{C}$ for which $Q = Q_q$ is positive. Since $\widetilde{q}(\mathcal{G})$ is a closed set, we have

$$q(\mathcal{G}) \subset \overline{q(\mathcal{G})} \subset \widetilde{q}(\mathcal{G}),$$

where $\overline{q(\mathcal{G})} \neq \widetilde{q}(\mathcal{G})$ may happen. Note also that $0 \in q(\mathcal{G})$ and $1 \in \widetilde{q}(\mathcal{G})$ for any graph $\mathcal{G}$. The next assertions are straightforward.

Proposition 3.2. *Let $\mathcal{G} = (V, E)$ be a graph with $|V| \geq 2$. Then $\widetilde{q}(\mathcal{G}) \subset [-1, 1]$ and $q(\mathcal{G}) \subset (-1, 1)$.*

Proposition 3.3. *If $\mathcal{G}$ is a finite graph, then $q(\mathcal{G})$ is an open subset of $(-1, 1)$ and $\widetilde{q}(\mathcal{G}) \setminus \overline{q(\mathcal{G})}$ consists of at most finitely many points.*

4. Detour join of two graphs. For $i = 1, 2$ let $\mathcal{G}_i = (V_i, E_i)$ be a graph with graph distance ∂_i. We assume that $V_1 \cap V_2 = \emptyset$. Let us consider a new graph $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ of the form

$$\widetilde{V} = V_1 \cup V_2, \qquad \widetilde{E} = E_1 \cup E_2 \cup E_{12}, \qquad E_{12} \subset \{\{x, y\}\,;\, x \in V_1,\ y \in V_2\}.$$

In this case $\mathcal{G}_i$ is an induced subgraph of $\widetilde{\mathcal{G}}$. Let $\widetilde{\partial}$ be the graph distance of $\widetilde{\mathcal{G}}$. We say that $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ is a *detour join* of $\mathcal{G}_1$ and $\mathcal{G}_2$ if

$$\widetilde{\partial}(x, y) = \partial_i(x, y), \qquad x, y \in V_i,$$

in other words, $\widetilde{\mathcal{G}}$ being regarded as an extension of $\mathcal{G}_i$, no properly shorter path is produced connecting $x, y \in V_i$ through vertices outside V_i.

Let $\widetilde{\mathcal{G}}=(\widetilde{V},\widetilde{E})$ be a *detour join* of $\mathcal{G}_1$ and $\mathcal{G}_2$ as above. Let Q_i be the Q-matrix of $\mathcal{G}_i$. Then the Q-matrix of $\widetilde{\mathcal{G}}$, denoted by $\widetilde{Q}$, is of the form

$$\widetilde{Q}=\left(\begin{array}{c|c} Q_1 & {}^tS \\ \hline S & Q_2 \end{array}\right), \tag{4.1}$$

where S is given by

$$S(y,x)=q^{\widetilde{\partial}(y,x)}, \quad y\in V_2,\, x\in V_1.$$

Being interested in positivity of $\widetilde{Q}$, in view of Proposition 3.2 we assume that $q\in[-1,1]$, and hence $\widetilde{Q}$ is a real symmetric matrix. From the expression (4.1) and the direct sum decomposition $C_0(V)\cong C_0(V_1)\oplus C_0(V_2)$, we may easily deduce the following

Lemma 4.1. *$\widetilde{Q}$ is positive if and only if*

$$\langle f_1,Q_1f_1\rangle+2\langle f_2,Sf_1\rangle+\langle f_2,Q_2f_2\rangle\geq 0$$

for all real $f_1\in C_0(V_1)$ and $f_2\in C_0(V_2)$. Moreover, $\widetilde{Q}$ is strictly positive if and only if

$$\langle f_1,Q_1f_1\rangle+2\langle f_2,Sf_1\rangle+\langle f_2,Q_2f_2\rangle> 0$$

for all real $f_1\in C_0(V_1)$ and $f_2\in C_0(V_2)$ with $(f_1,f_2)\neq(0,0)$.

Then by an elementary argument using discriminants we obtain

Proposition 4.2. *$\widetilde{Q}$ is positive if and only if both Q_1 and Q_2 are positive and*

$$\langle f_2,Sf_1\rangle^2\leq\langle f_1,Q_1f_1\rangle\langle f_2,Q_2f_2\rangle$$

for all real $f_1\in C_0(V_1)$ and $f_2\in C_0(V_2)$. Moreover, $\widetilde{Q}$ is strictly positive if and only if both Q_1 and Q_2 are strictly positive and

$$\langle f_2,Sf_1\rangle^2<\langle f_1,Q_1f_1\rangle\langle f_2,Q_2f_2\rangle$$

for all real $f_1\in C_0(V_1)$ and $f_2\in C_0(V_2)$ with $f_1\neq 0$, $f_2\neq 0$.

Corollary 4.3. *$\widetilde{q}(\widetilde{Q})\subset\widetilde{q}(Q_1)\cap\widetilde{q}(Q_2)$ and $q(\widetilde{Q})\subset q(Q_1)\cap q(Q_2)$.*

Although Proposition 4.2 covers a general detour join, checking the inequalities therein seems to be practically difficult.

We now focus on a special case. Given a graph $\mathcal{G}=(V,E)$, let $\widetilde{\mathcal{G}}=(\widetilde{V},\widetilde{E})$ be a new graph defined by

$$\widetilde{V}=V\cup\{o\}, \qquad \widetilde{E}=E\cup E_o, \qquad E_o\subset\{\{o,x\}\,;\,x\in V\}.$$

As is easily verified, $\widetilde{\mathcal{G}}$ is a detour join of $\mathcal{G}$ with the trivial graph $(\{o\},\emptyset)$ if and only if $\partial(x,y)\leq 2$ for all $x,y\in V$ such that $\{o,x\},\{o,y\}\in E_o$, where ∂ is the graph distance of $\mathcal{G}$. In this case, $\widetilde{\mathcal{G}}$ is called a *one-vertex detour extension* of $\mathcal{G}$. Then the matrix S in (4.1) becomes a column vector with index set V whose xth element is $q^{\widetilde{\partial}(x,o)}$. As a direct consequence of Proposition 4.2 we obtain

THEOREM 4.4. *Let $\widetilde{\mathcal{G}}$ be a one-vertex detour extension of $\mathcal{G} = (V, E)$. Let $\widetilde{Q}$ and Q denote the Q-matrices of $\widetilde{\mathcal{G}}$ and $\mathcal{G}$, respectively. Then $\widetilde{Q}$ is positive if and only if Q is positive and*

$$\langle f, S\rangle^2 \le \langle f, Qf\rangle$$

for all real $f \in C_0(V)$. Similarly, $\widetilde{Q}$ is strictly positive if and only if Q is strictly positive and

$$\langle f, S\rangle^2 < \langle f, Qf\rangle$$

for all real $f \in C_0(V)$ with $f \neq 0$.

COROLLARY 4.5. *Let $\widetilde{\mathcal{G}}$ be a one-vertex detour extension of $\mathcal{G}$. Let $\widetilde{Q}$ and Q denote the Q-matrices of $\widetilde{\mathcal{G}}$ and $\mathcal{G}$, respectively. Then $\widetilde{q}(\widetilde{Q}) \subset \widetilde{q}(Q)$ and $q(\widetilde{Q}) \subset q(Q)$.*

REMARK 4.6. Assume that V is finite. Let P_S be the projection onto the one-dimensional subspace of $C(V)$ spanned by S. Since

$$\langle f, S\rangle^2 = \langle S, S\rangle\langle f, P_S f\rangle, \qquad f \in C(V),$$

the inequalities mentioned in Theorem 4.4 can be rephrased in terms of positivity of $Q - \langle S, S\rangle P_S$.

We consider a further special case. Given a graph $\mathcal{G} = (V, E)$, taking $a \in V$ and a new vertex o we define a new graph $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ by

$$\widetilde{V} = V \cup \{o\}, \qquad \widetilde{E} = E \cup \{\{o, a\}\}.$$

Obviously, $\widetilde{\mathcal{G}}$ becomes a one-vertex detour extension of $\mathcal{G}$. This special case is referred to as *segment-concatenation*.

THEOREM 4.7. *If $\widetilde{\mathcal{G}}$ is a segment-concatenation of $\mathcal{G}$, we have $\widetilde{q}(\widetilde{\mathcal{G}}) = \widetilde{q}(\mathcal{G})$ and $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$.*

Since $\widetilde{\mathcal{G}}$ is a star product of $\mathcal{G}$ and a segment C^2, the assertion is just a special case of Theorem 1.1. Alternatively, the conditions in Theorem 4.4 can be verified directly. The latter observation, in fact, leads to the main theorem of this paper.

5. Joining a square. We now consider extending a graph $\mathcal{G} = (V, E)$ by joining a square. We consider three cases, as stated in the introduction (see also Figure 1 therein).

CASE 1: *One-vertex detour extension making a square.* Taking $a, b \in V$ with $\partial(a, b) = 2$ and a new vertex o, we define a graph $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ by

$$\widetilde{V} = V \cup \{o\}, \qquad \widetilde{E} = E \cup \{\{o, a\}, \{o, b\}\}. \tag{5.1}$$

Case 2: *Square-concatenation.* Taking $b, c \in V$ with $\partial(b,c) = 1$ and new vertices o, a, we define a graph $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ by

$$\widetilde{V} = V \cup \{o, a\}, \qquad \widetilde{E} = E \cup \{\{o,a\}, \{o,b\}, \{a,c\}\}.$$

Case 3: *Star product with a square.* Taking $c \in V$ and new vertices o, a, b, we define a graph $\widetilde{\mathcal{G}} = (\widetilde{V}, \widetilde{E})$ by

$$\widetilde{V} = V \cup \{o, a, b\}, \qquad \widetilde{E} = E \cup \{\{o,a\}, \{o,b\}, \{a,c\}, \{b,c\}\}.$$

These are all particular cases of detour join of two graphs. In Case 1, $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$ does not hold in general. In Section 5.1 we shall prove the equality under a certain condition. The equality $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$ holds in Cases 2 and 3. Case 2 will be discussed in Section 5.2. Case 3 reduces to Theorem 1.1, as explained in the introduction. Thus the main theorem stated in the introduction follows.

5.1. *One-vertex detour extension making a square.* We maintain the notations and assumptions stated in Case 1. Set

$$\begin{aligned} V_a &= \{x \in V \,;\, \partial(x,a) < \partial(x,b)\}, \\ V_b &= \{x \in V \,;\, \partial(x,b) < \partial(x,a)\}, \\ V' &= \{x \in V \,;\, \partial(x,a) = \partial(x,b)\}. \end{aligned}$$

Then $V = V_a \cup V_b \cup V'$ is a partition. Note also that $a \in V_a$ and $b \in V_b$.

Lemma 5.1. *Let $x \in V_a$. Then every shortest path in $\widetilde{\mathcal{G}}$ from x to o is of the form $x \sim \cdots \sim a \sim o$, that is, it passes through the vertex a just before reaching o. A parallel statement for $y \in V_b$ is also valid.*

Lemma 5.2. *Let $x \in V'$. There exists a shortest path in $\widetilde{\mathcal{G}}$ connecting x and o of the form $x \sim \cdots \sim a \sim o$ as well as one of the form $x \sim \cdots \sim b \sim o$.*

Lemma 5.3. *For $x \in V$ we have*

$$\widetilde{\partial}(x,o) = \begin{cases} \partial(x,a) + 1, & x \in V_a, \\ \partial(x,b) + 1, & x \in V_b, \\ \partial(x,a) + 1 = \partial(x,b) + 1, & x \in V'. \end{cases}$$

The proofs of the lemmata above are straightforward. We now consider the essential condition on the choice of vertices a, b of $\mathcal{G}$:

(H) There exists $c \in V$ such that

   (i) $\partial(c,a) = \partial(c,b) = 1$;

   (ii) for any $x \in V$ with $\partial(x,b) \le \partial(x,a)$, there exists a shortest path from x to a passing through c, in other words,

$$\partial(x,a) = \partial(x,c) + 1, \qquad x \in V_b \cup V';$$

(iii) for any $y \in V$ with $\partial(y,a) \le \partial(y,b)$, there exists a shortest path from y to b passing through c, in other words,

$$\partial(y,b) = \partial(y,c) + 1, \qquad y \in V_a \cup V'.$$

If $\widetilde{\mathcal{G}}$ is obtained by a one-vertex detour extension making a square and satisfying condition (H), we call it *admissible.*

THEOREM 5.4. *If $\widetilde{\mathcal{G}}$ is obtained from a finite graph $\mathcal{G}$ by an admissible one-vertex detour extension making a square, then $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$.*

Proof. The Q-matrices of $\mathcal{G}$ and $\widetilde{\mathcal{G}}$ are denoted by Q and $\widetilde{Q}$, respectively. By Corollary 4.5, it is sufficient to show that $q(\widetilde{\mathcal{G}}) \supset q(\mathcal{G})$, or equivalently that $\widetilde{Q}$ is strictly positive for $q \in q(\mathcal{G})$. Keeping in mind the partition

$$\widetilde{V} = V \cup \{o\} = V_a \cup V_b \cup V' \cup \{o\},$$

we fix a decreasing sequence

$$\widetilde{V} = U_n \supset U_{n-1} \supset \cdots \supset U_4 \supset U_3 \supset U_2 \supset U_1$$

satisfying

$$|U_s \setminus U_{s-1}| = 1, \qquad s = 2, \dots, n,$$

and

$$U_4 = \{a,b,c,o\}, \quad U_3 = \{a,b,c\}, \quad U_2 = \{a,c\}, \quad U_1 = \{a\}.$$

We set

$$\Delta_s = \det \widetilde{Q}\restriction U_s, \qquad s = 1, \dots, n. \tag{5.2}$$

Then, by Proposition 2.6, to prove that $\widetilde{Q}$ is strictly positive it is sufficient to show that

$$\Delta_s > 0, \qquad s = 1, \dots, n, \tag{5.3}$$

whenever Q is strictly positive, i.e., $q \in q(Q)$.

Let us compute Δ_s in (5.2) explicitly. The first four are easily obtained:

$$\Delta_1 = 1, \tag{5.4}$$

$$\Delta_2 = \det \begin{pmatrix} 1 & q \\ q & 1 \end{pmatrix} = 1 - q^2, \tag{5.5}$$

$$\Delta_3 = \det \begin{pmatrix} 1 & q^2 & q \\ q^2 & 1 & q \\ q & q & 1 \end{pmatrix} = (1-q^2)^2, \tag{5.6}$$

$$\Delta_4 = \det \begin{pmatrix} 1 & q & q & q^2 \\ q & 1 & q^2 & q \\ q & q^2 & 1 & q \\ q^2 & q & q & 1 \end{pmatrix} = (1-q^2)^4. \tag{5.7}$$

Let $5 \le s \le n$. Note that $\{o,a,b,c\} \subset U_s$. Consider a matrix R obtained from $\widetilde{Q}\restriction U_s$ by subtracting q times the bth column from the oth column. Then the elements of R are given by

$$R(x,o) = \widetilde{Q}(x,o) - q\widetilde{Q}(x,b) = q^{\widetilde{\partial}(x,o)} - qq^{\partial(x,b)}, \quad x \in U_s,$$
$$R(x,y) = \widetilde{Q}(x,y) = q^{\widetilde{\partial}(x,y)}, \quad x \in U_s,\ y \in U_s \setminus \{o\}.$$

In particular,

$$R(o,o) = 1-q^2, \qquad R(a,o) = q-q^3, \tag{5.8}$$

and, using Lemma 5.3,

$$\begin{aligned} R(x,o) &= q^{\widetilde{\partial}(x,o)} - qq^{\partial(x,b)} \\ &= q^{\partial(x,b)+1} - qq^{\partial(x,b)} = 0, \quad x \in (V_b \cup V') \cap U_s. \end{aligned} \tag{5.9}$$

Next let R' denote the matrix obtained from R by subtracting q times the ath row from the oth row. Then

$$R'(o,y) = R(o,y) - qR(a,y), \qquad y \in U_s,$$
$$R'(x,y) = R(x,y), \qquad x \in U_s \setminus \{o\},\ y \in U_s.$$

In particular,

$$R'(o,o) = R(o,o) - qR(a,o) = (1-q^2)^2, \tag{5.10}$$

$$R'(o,y) = q^{\widetilde{\partial}(o,y)} - qq^{\partial(a,y)}, \qquad y \in U_s \setminus \{o\}. \tag{5.11}$$

Moreover, since $R'(x,o) = R(x,o)$ for $x \in U_s \setminus \{o\}$, we see from (5.9) that

$$R'(x,o) = 0, \quad x \in (V_b \cup V') \cap U_s. \tag{5.12}$$

Let ϱ'_x denote the (x,o)-cofactor of R'. Then

$$\Delta_s = \det R = \det R' = \sum_{x \in U_s} R'(x,o)\varrho'_x.$$

In view of (5.10) and (5.12) we obtain

$$\Delta_s = (1-q^2)^2 \varrho'_o + \sum_{x \in V_a \cap U_s} R'(x,o)\varrho'_x. \tag{5.13}$$

Let R'_x denote the submatrix obtained from R' by deleting the xth row and the oth column. Then by construction we have

$$\varrho'_o = \det R'_o = \det \widetilde{Q}\restriction U_s \setminus \{o\} = \det Q \restriction U_s \setminus \{o\}. \tag{5.14}$$

We shall show that

$$\varrho'_x = 0, \qquad x \in V_a \cap U_s. \tag{5.15}$$

Since ϱ'_x coincides with $\det R'_x$ up to sign, it is sufficient to show that $\det R'_x = 0$ for $x \in V_a \cap U_s$. This will be proved by showing that the rows of R'_x are not linearly independent. We prove that

$$(o\text{th row}) = q((b\text{th row}) - q(c\text{th row})),$$

in other words,

$$R'_x(o, y) = q(R'_x(b, y) - qR'_x(c, y)), \qquad y \in U_s \setminus \{o\}. \tag{5.16}$$

In fact, the left hand side becomes

$$R'_x(o, y) = R'(o, y) = q^{\widetilde{\partial}(o,y)} - qq^{\partial(a,y)}.$$

If $y \in V_b$, using $\partial(y, a) = \partial(y, c) + 1$ in condition (H), we have

$$\begin{aligned} R'_x(o, y) &= q^{\widetilde{\partial}(o,b)+\partial(b,y)} - qq^{\partial(c,y)+1} = q(q^{\partial(b,y)} - qq^{\partial(c,y)}) \\ &= q(R'_x(b, y) - qR'_x(c, y)), \end{aligned}$$

which proves (5.16) for $y \in V_b$. Let $y \in V_a \cup V'$. Since $\widetilde{\partial}(o, y) = \partial(a, y) + 1$ by Lemma 5.3, we have

$$R'_x(o, y) = q^{\widetilde{\partial}(o,y)} - qq^{\partial(a,y)} = 0. \tag{5.17}$$

On the other hand, since $\partial(y, b) = \partial(y, c) + 1$ by condition (H), we have

$$R'_x(b, y) - qR'_x(c, y) = q^{\partial(b,y)} - qq^{\partial(c,y)} = 0. \tag{5.18}$$

We see from (5.17) and (5.18) that (5.16) holds for $y \in V_a \cup V'$ too, which completes the proof of (5.16).

Consequently, by combining (5.13)–(5.15), we come to

$$\Delta_s = (1 - q^2)^2 \det Q{\restriction}U_s \setminus \{o\}, \quad s = 5, \dots, n. \tag{5.19}$$

In view of the explicit forms of Δ_s in (5.4)–(5.7) and (5.19) together with the assumption $q \in q(\mathcal{G}) \subset (-1, 1)$, we obtain our goal (5.3). ∎

5.2. *Square-concatenation.* We maintain the notations and assumptions stated in Case 2. The graph $\widetilde{\mathcal{G}}$ therein is called a *square-concatenation* of $\mathcal{G}$.

THEOREM 5.5. *If $\widetilde{\mathcal{G}}$ is a square-concatenation of a finite graph $\mathcal{G}$, then $q(\widetilde{\mathcal{G}}) = q(\mathcal{G})$.*

Proof. The square-concatenation is divided into two steps (see Figure 1(2)). We define an intermediate graph $\mathcal{H} = (W, F)$ by

$$W = V \cup \{a\}, \qquad F = E \cup \{\{a, c\}\}.$$

That is, $\mathcal{H}$ is a segment-concatenation of $\mathcal{G}$. By Theorem 4.7 we know that $q(\mathcal{H}) = q(\mathcal{G})$. Next we note that $\widetilde{\mathcal{G}}$ is a one-vertex detour extension of $\mathcal{H}$

considered in Case 1. Provided condition (H) is satisfied, it follows from Theorem 5.4 that $q(\widetilde{\mathcal{G}}) = q(\mathcal{H})$, and our assertion follows.

We now prove that the vertex c of $\mathcal{H} = (W, F)$ satisfies the condition in (H). The graph distance of $\mathcal{H}$ is denoted by ∂. Set

$$W_a = \{x \in W\,;\, \partial(x,a) < \partial(x,b)\},$$
$$W_b = \{x \in W\,;\, \partial(x,a) > \partial(x,b)\},$$
$$W' = \{x \in W\,;\, \partial(x,a) = \partial(x,b)\}.$$

By construction of the graph $\mathcal{H}$, every path from an arbitrary $x \in W_b \cup W'$ to a passes through c, so that condition (H-ii) is obvious. Let $y \in W_a \cup W'$, that is,

$$\partial(y,a) \le \partial(y,b). \tag{5.20}$$

Take a shortest path from y to a, which is of the form $y \sim \cdots \sim c \sim a$. Then $y \sim \cdots \sim c \sim b$ becomes a path connecting y and b with length $\partial(y,a)$. Due to the inequality (5.20) this is a shortest path, which certainly passes through c. Thus condition (H-iii) is proved. ∎

6. Concrete examples

6.1. *Integer lattice* $\mathbb{Z}^2$

THEOREM 6.1. *$q(\mathbb{Z}^2) = (-1,1)$ and $\widetilde{q}(\mathbb{Z}^2) = [-1,1]$.*

Proof. Let Q denote the Q-matrix of $\mathbb{Z}^2$. For $N = 1, 2, \dots$ set

$$V_N = \{(m,n) \in \mathbb{Z}^2\,;\, |m| \le N,\ |n| \le N\}$$

and let $\mathcal{G}_N$ be the induced subgraph of $\mathbb{Z}^2$ whose vertex set is V_N, i.e., $\mathcal{G}_N$ is a finite lattice of size $2N \times 2N$. Obviously, the Q-matrix of $\mathcal{G}_N$ coincides with $Q \restriction V_N$. On the other hand, it is easy to see that $\mathcal{G}_N$ is obtained from a square C^4 by repeated application of admissible one-vertex detour extension and square-concatenation. Hence

$$q(Q \restriction V_N) = q(C^4) = (-1,1). \tag{6.1}$$

Let $q \in (-1,1)$ and take $f \in C_0(\mathbb{Z}^2)$, $f \ne 0$. Choosing $N \ge 1$ sufficiently large, we have

$$\langle f, Qf \rangle = \sum_{x,y \in V_N} f(x) q^{\partial(x,y)} f(y) = \langle f \restriction V_N, (Q \restriction V_N)(f \restriction V_N) \rangle > 0$$

by (6.1). Hence Q is strictly positive. Consequently, $q(\mathbb{Z}^2) = (-1,1)$. The second assertion is then immediate. ∎

Many subgraphs $\mathcal{G} \subset \mathbb{Z}^2$ with $q(\mathcal{G}) = (-1,1)$ can be constructed by repeated application of the three extensions mentioned in the main theorem.

6.2. *Cyclic graph C^{2n}.* For $n = 2, 3, \ldots$ let C^{2n} denote the cyclic graph with $2n$ vertices. By convention C^2 denotes a graph with two vertices and one edge.

THEOREM 6.2. *For $n = 1, 2, 3, \ldots$ we have*

$$q(C^{2n}) = (-1, 1), \qquad \widetilde{q}(C^{2n}) = [-1, 1].$$

Proof. We only consider the case of $n \geq 2$. We set $C^{2n} = (V, E)$, where

$$V = \{0, 1, 2, \ldots, 2n-1\}, \quad E = \{\{0,1\}, \{1,2\}, \ldots, \{2n-1, 0\}\}.$$

Let W be a permutation matrix acting on V as $0 \to 1 \to \cdots \to 2n-1 \to 0$. Then

$$Q = 1 + \sum_{j=1}^{n-1} q^j (W^j + W^{-j}) + q^n W^n. \tag{6.2}$$

Using the eigenvalues and eigenvectors of W explicitly, we obtain the full description of the eigenvalues of Q as follows:

$$\lambda_0 = \frac{(1-q^n)(1+q)}{1-q}, \qquad \lambda_n = \frac{(1+(-1)^{n+1}q^n)(1-q)}{1+q}$$

are the eigenvalues of multiplicity one, and

$$\lambda_k = \frac{(1+(-1)^{k+1}q^n)(1-q^2)}{|1-q\omega^k|^2}, \qquad 1 \leq k \leq n-1,$$

are the ones of multiplicity two, where $\omega = \exp\left(\frac{2\pi i}{2n}\right)$ is the primitive $2n$-root of one. All the eigenvalues are positive, equivalently Q is strictly positive if and only if $-1 < q < 1$. By continuity Q is positive for $-1 \leq q \leq 1$. ∎

6.3. *Cyclic graph C^{2n+1}.* The situation for a cyclic graph with an odd number of vertices is slightly more complicated. To state the result we need to define a sequence $\{r_n\,;\, n = 1, 2, \ldots\}$. For any odd integer $n = 1, 3, 5, \ldots$ the algebraic equation

$$f_n(r) = 1 + r - 2r^{n+1} = 0$$

has a unique negative root (in fact this root lies in $(-1, 0)$), which we denote by r_n. For any even integer $n = 2, 4, \ldots$ the algebraic equation

$$f_n(r) = 1 + r + 2r^{n+1} \cos\frac{\pi}{2n+1} = 0$$

has a unique real root (in fact the root is found in $(-1, 0)$), which we also denote by r_n. It is an elementary observation that

$$-1/2 = r_1 > r_2 > \cdots \to -1.$$

THEOREM 6.3. *Let $n = 1, 2, \ldots$ and r_n as above. We have*

$$q(C^{2n+1}) = (r_n, 1), \qquad \widetilde{q}(C^{2n+1}) = [r_n, 1].$$

Proof. Employing similar notations to those in the proof of Theorem 6.2, we have

$$Q = 1 + \sum_{j=1}^{n} q^j (W^j + W^{-j}),$$

where W is the permutation matrix acting on $V = \{0, 1, 2, \dots, 2n\}$ as $0 \to 1 \to \cdots \to 2n \to 0$. Then the eigenvalues of Q are easily obtained:

$$\lambda_k = \frac{1-q}{|1-q\omega^k|^2} \left(1 + q - 2q^{n+1} \cos \frac{2kn}{2n+1}\pi \right), \qquad 0 \le k \le 2n,$$

where $\omega = \exp\left(\frac{2\pi i}{2n+1}\right)$ is the primitive $(2n+1)$-root of one. Note that $\lambda_k = \lambda_{2n+1-k}$. If $0 < q < 1$, we have

$$\lambda_0 < \lambda_1 < \cdots < \lambda_n. \tag{6.3}$$

If $-1 < q < 0$ and n is odd, (6.3) remains valid. If $-1 < q < 0$ and n is even, we have

$$\lambda_0 > \lambda_1 > \cdots > \lambda_n. \tag{6.4}$$

Consequently, all the eigenvalues of Q are positive if and only if $\lambda_0 > 0$ or $\lambda_n > 0$ according as n is odd or even. ∎

Corollary 6.4. *If a graph $\mathcal{G}$ contains a triangle, then*

$$q(\mathcal{G}) \subset (-1/2, 1), \qquad \widetilde{q}(\mathcal{G}) \subset [-1/2, 1].$$

6.4. *Complete graph K_n.* A graph is called *complete* if every pair of vertices is connected by an edge. A complete graph with n vertices is denoted by K_n.

Theorem 6.5. *For $n \ge 2$ we have*

$$q(K_n) = \left(-\frac{1}{n-1}, 1 \right), \qquad \widetilde{q}(K_n) = \left[-\frac{1}{n-1}, 1 \right].$$

Proof. The eigenvalues of the Q-matrix of K_n are easily computed:

$$(1-q) + qn \quad (\text{multiplicity } 1), \qquad 1 - q \quad (\text{multiplicity } n-1),$$

from which the assertion is immediate. ∎

Remark 6.6. Let Q_n denote the Q-matrix of K_n. The principal submatrices of Q_n are $Q_1, \dots, Q_n$ and their determinants are easily computed:

$$\det Q_s = (1-q)^{s-1}(1 + (s-1)q).$$

Thus $q(K_n)$ and $\widetilde{q}(K_n)$ can also be obtained from

$$q(K_n) = \{q \in (-1, 1)\,;\, (1-q)^{s-1}(1 + (s-1)q) > 0 \text{ for all } s = 1, \dots, m\},$$
$$\widetilde{q}(K_n) = \{q \in [-1, 1]\,;\, (1-q)^{s-1}(1 + (s-1)q) \ge 0 \text{ for all } s = 1, \dots, m\}.$$

6.5. *Complete bipartite graph $K_{m,n}$.* Let $m \geq 1$, $n \geq 1$ be a pair of integers. A graph $\mathcal{G} = (V, E)$ is called *completely bipartite*, and is denoted by $K_{m,n}$, if V admits a partition

$$V = U_m \cup U_n,$$

where U_m and U_n respectively consist of m and n vertices, and

$$E = \{\{x, y\}\,;\, x \in U_m,\ y \in U_n\}.$$

Without loss of generality we may assume that $1 \leq m \leq n$. If $m = 1$, the complete bipartite graph $K_{1,n}$ is called a *star graph*.

The Q-matrix of $K_{m,n}$ is denoted by $Q_{m,n}$ in this subsection. Its explicit form is

$$Q_{m,n} = \left(\begin{array}{c|c} R_m & S_{m,n} \\ \hline S_{n,m} & R_n \end{array}\right),$$

where the $m \times m$ matrix R_m and the $m \times n$ matrix $S_{m,n}$ are defined by

$$R_m = \begin{pmatrix} 1 & q^2 & \dots & q^2 \\ q^2 & 1 & \dots & q^2 \\ \vdots & \vdots & \ddots & \vdots \\ q^2 & q^2 & \dots & 1 \end{pmatrix}, \qquad S_{m,n} = \begin{pmatrix} q & q & \dots & q \\ q & q & \dots & q \\ \vdots & \vdots & \ddots & \vdots \\ q & q & \dots & q \end{pmatrix}.$$

Positivity or strict positivity of $Q_{m,n}$ may be determined from its principal minors.

For $s = 1, \dots, m+n$ let Δ_s be the sth principal minor of $Q_{m,n}$, i.e.,

$$\Delta_1 = \det R_1, \quad \dots, \quad \Delta_n = \det R_n,$$
$$\Delta_{1+n} = \det Q_{1,n}, \quad \dots, \quad \Delta_{m+n} = \det Q_{m,n}.$$

By elementary linear algebra, $Q_{m,n}$ is strictly positive if and only if $\Delta_s > 0$ for all $1 \leq s \leq m+n$. The relevant determinants are easily calculated:

$$\det R_s = \det \begin{pmatrix} 1 & q^2 & \dots & q^2 \\ q^2 & 1 & \dots & q^2 \\ \vdots & \vdots & \ddots & \vdots \\ q^2 & q^2 & \dots & 1 \end{pmatrix} = (1 + (s-1)q^2)(1 - q^2)^{s-1}, \tag{6.5}$$

$$\det Q_{1,n} = \det \left(\begin{array}{c|cccc} 1 & q & q & \dots & q \\ \hline q & 1 & q^2 & \dots & q^2 \\ q & q^2 & 1 & \dots & q^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ q & q^2 & q^2 & \dots & 1 \end{array}\right) = (1 - q^2)^n, \tag{6.6}$$

$$\det Q_{m,n} = (1-(m-1)(n-1)q^2)(1-q^2)^{m+n-1}, \qquad m \ge 2. \tag{6.7}$$

Thus, strict positivity of $Q_{m,n}$ is seen from (6.5)–(6.7). On the other hand, $Q_{m,n}$ is positive if and only if all principal minors are non-negative. Since any principal minor is of the form $\det R_s$ or $\det Q_{s,t}$, the verification also reduces to (6.5)–(6.7). Thus we come to the following

THEOREM 6.7. *For the star graph $K_{1,n}$, $n \ge 1$, we have*

$$q(K_{1,n}) = (-1,1), \qquad \widetilde{q}(K_{1,n}) = [-1,1].$$

THEOREM 6.8. *Let $2 \le m \le n$. Then*

$$q(K_{m,n}) = \left(-\frac{1}{\sqrt{(m-1)(n-1)}}, \frac{1}{\sqrt{(m-1)(n-1)}}\right),$$

$$\widetilde{q}(K_{m,n}) = \left[-\frac{1}{\sqrt{(m-1)(n-1)}}, \frac{1}{\sqrt{(m-1)(n-1)}}\right] \cup \{-1,1\}.$$

References

[1] N. Biggs, *Algebraic Graph Theory*, 2nd ed., Cambridge Univ. Press, 1993.

[2] M. Bożejko, *Uniformly bounded representations of free groups*, J. Reine Angew. Math. 377 (1987), 170–186.

[3] —, *Positive-definite kernels, length functions on groups and noncommutative von Neumann inequality*, Studia Math. 95 (1989), 107–118.

[4] M. Bożejko, T. Januszkiewicz and R. J. Spatzier, *Infinite Coxeter groups do not have Kazhdan's property*, J. Operator Theory 19 (1988), 63–67.

[5] M. Bożejko and R. Szwarc, *Algebraic length and Poincaré series on reflection groups with applications to representation theory*, in: Asymptotic Combinatorics with Applications to Mathematical Physics, A. M. Vershik (ed.), Lecture Notes in Math. 1815, Springer, Berlin, 2003, 201–221.

[6] D. M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs*, Academic Press, 1979.

[7] D. Ž. Djoković, *Distance-preserving subgraphs of hypercubes*, J. Combin. Theory Ser. B 14 (1973), 263–267.

[8] A. Figà-Talamanca and M. A. Picardello, *Harmonic Analysis on Free Groups*, Lecture Notes in Pure and Appl. Math. 87, Dekker, 1983.

[9] U. Haagerup, *An example of a nonnuclear C^*-algebra which has the metric approximation property*, Invent. Math. 50 (1979), 279–293.

[10] A. Hora, *Gibbs state on a distance-regular graph and its application to a scaling limit of the spectral distributions of discrete Laplacians*, Probab. Theory Related Fields 118 (2000), 115–130.

[11] A. Hora and N. Obata, *Asymptotic spectral analysis of growing regular graphs*, Trans. Amer. Math. Soc., to appear.

[12] —, —, *Quantum Probability and Spectral Analysis of Graphs*, Springer, to appear.

[13] N. Obata, *Quantum probabilistic approach to spectral analysis of star graphs*, Interdiscip. Inform. Sci. 10 (2004), 41–52.

[14] B. Simon, *Operators with singular continuous spectrum, VI. Graph Laplacians and Laplace–Beltrami operators*, Proc. Amer. Math. Soc. 124 (1996), 1177–1182.

Graduate School of Information Sciences
Tohoku University
Sendai 980-8579, Japan
E-mail: obata@math.is.tohoku.ac.jp

Received May 1, 2006
Revised version October 20, 2006 (5911)