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MARKOV PRODUCT OF POSITIVE DEFINITE KERNELS AND APPLICATIONS TO Q-MATRICES OF GRAPH PRODUCTS

BY

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Abstract. We show positivity of the Q-matrix of four kinds of graph products: direct product (Cartesian product), star product, comb product, and free product. During the discussion we give an alternative simple proof of the Markov product theorem on positive definite kernels.

1. Introduction. This short paper is motivated by the elegant result on positive definite kernels due to Bożejko [3]. Although his result is more general on operator-valued kernels, keeping our purpose in mind we state it in the following form:

THEOREM 1.1 (Bożejko). *Let V be a (finite or infinite) set which is the union of two subsets V_1, V_2 whose intersection consists of a single point, say $o \in V$:*

$$V = V_1 \cup V_2\,, \qquad V_1 \cap V_2 = \{o\}.$$

For $i = 1, 2$ let K_i be a positive definite (resp. strictly positive definite) kernel on V_i and assume that $K_1(o,o) = K_2(o,o) = 1$. Then the $\mathbb{C}$-valued function K on $V \times V$ defined by

$$K(x,y) = \begin{cases} K_1(x,y) & \text{if } x,y \in V_1, \\ K_2(x,y) & \text{if } x,y \in V_2, \\ K_1(x,o)K_2(o,y) & \text{if } x \in V_1,\ y \in V_2, \\ K_2(x,o)K_1(o,y) & \text{if } x \in V_2,\ y \in V_1, \end{cases}$$

is a positive definite (resp. strictly positive definite) kernel on V.

The positive definite kernel K defined in the above theorem is called the *Markov product* of K_1 and K_2. There are many applications. For example, positivity of the Haagerup states [9] on a free group follows as a direct consequence. Being valid for an arbitrary underlying set and for positive

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definite operator-valued kernels, Bożejko's theorem unifies various results on positive definite kernels (see [3]).

As is well known, various matrices associated with a graph, e.g., the adjacency matrix, distance matrix, incidence matrix, Laplacian, transition matrix and so forth, are keys for algebraic, analytic, or probabilistic approaches to the structural study of graphs (see e.g., [2, 4, 5, 6, 16] and references cited therein). The Q-matrix of a graph $G = (V, E)$, defined by

$$Q = Q(G; q) = [q^{\partial_G(x,y)}]_{x,y \in V}, \qquad q \in \mathbb{C},$$

where $\partial_G(x, y)$ stands for the graph distance between two vertices, is also worthy of attention. It defines the q-deformed vacuum states and plays an interesting role in (asymptotic) spectral analysis of graphs along with quantum probability theory [10, 11, 12]. However, positivity of the Q-matrix is a difficult question in general and so a systematic approach is desirable. The detour join of two graphs is one of the attempts [15]. In this paper we discuss the positivity of the Q-matrix in connection with four kinds of graph products: direct product (Cartesian product), star product, comb product and free product. It is noteworthy that these four graph products are related to four concepts of independence in quantum probability theory, namely, commutative independence, Boolean independence, monotone independence, and free independence (see, e.g., [11]).

This paper is organized as follows: In Section 2 we collect basic notions and notations. In Section 3 we give an alternative simple proof of Bożejko's theorem. In Section 4 we recall basic properties of Q-matrices. Finally in Section 5 we prove the positivity of the Q-matrices of graph products.

2. Positive definite kernels. In order to avoid confusion we assemble some notions and notations. Let V be a non-empty (finite or infinite) set. We denote by $C(V)$ the space of $\mathbb{C}$-valued functions on V and by $C_0(V)$ the subspace of those with finite supports. For $f, g \in C(V)$ we define

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

whenever the sum is absolutely convergent. We always assume that $C_0(V)$ is a pre-Hilbert space equipped with the inner product defined above.

A $\mathbb{C}$-valued function K defined on $V \times V$ is called a *kernel* on V. A kernel K is identified with a linear operator from $C_0(V)$ into $C(V)$ (denoted by the same symbol) in the usual manner:

$$Kf(x) = \sum_{y \in V} K(x, y) f(y), \qquad f \in C_0(V).$$

Motivated by the above expression, we sometimes employ a matrix representation $K = [K(x, y)]_{x,y \in V}$.

DEFINITION 2.1. A kernel K is called *positive definite* (abbr. pd) if

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

It is called *strictly positive definite* (abbr. spd) if

$$\langle f, Kf \rangle = \sum_{x,y \in V} \overline{f(x)}\, K(x,y) f(y) > 0 \quad \text{for all } f \in C_0(V),\ f \neq 0.$$

Let K be a kernel on V. For a non-empty subset $W \subset V$, we denote by $K\restriction_W$ the restriction of K to $W \times W$. Obviously, if K is a pd (or spd) kernel, then so are all restrictions. In particular, if W is a finite set, $K\restriction_W$ is regarded as a positive definite (resp. strictly positive definite) matrix and hence it is hermitian symmetric with non-negative (resp. positive) eigenvalues.

The following criterion, which is straightforward by definition, will be repeatedly used below.

LEMMA 2.2. *A kernel K on V is pd (resp. spd) if there exists a sequence of finite subsets $W_1 \subset W_2 \subset \cdots \subset V$ with $V = \bigcup_n W_n$ such that $K\restriction_{W_n}$ is pd (resp. spd) for all $n = 1, 2, \ldots$.*

For further properties of positive definite kernels, see, e.g., [7, 13].

3. A simple proof of Theorem 1.1. Let K_1 and K_2 be kernels on V_1 and V_2, respectively. The tensor product $K_1 \otimes K_2$ is a kernel on $V_1 \times V_2$ defined by

$$(K_1 \otimes K_2)((x_1, y_1), (x_2, y_2)) = K_1(x_1, x_2) K_2(y_1, y_2)$$

for $(x_1, y_1), (x_2, y_2) \in V_1 \times V_2$. Note that $K_1 \otimes K_2$ is identified with a linear operator from $C_0(V_1) \otimes C_0(V_2) \cong C_0(V_1 \times V_2)$ into $C(V_1 \times V_2)$.

We start with the following fairly obvious result.

THEOREM 3.1. *Let K_1 and K_2 be pd (resp. spd) kernels on V_1 and V_2, respectively. Then $K = K_1 \otimes K_2$ is a pd (resp. spd) kernel on $V = V_1 \times V_2$.*

Proof. By Lemma 2.2, it is sufficient to prove the assertion when V_1 and V_2 are finite sets, i.e., when K_1 and K_2 are matrices (of finite orders). But the assertion for matrices is well known and easy to show, for example by diagonalization (see, e.g., [13, Chap. 4]). ∎

Proof of Theorem 1.1. We only prove the case where K_1 and K_2 are positive definite kernels on V_1 and V_2, respectively. The argument for strictly positive definite kernels is parallel. Let $X = V_1 \times V_2$ and set

$$\tilde{V} = \{(x, o_2) : x \in V_1\} \cup \{(o_1, y) : y \in V_2\}.$$

Since $K_1 \otimes K_2$ becomes a positive definite kernel on X by Theorem 3.1, so is the restriction $(K_1 \otimes K_2)\restriction_{\tilde{V}}$. On the other hand, through the natural bijection between $\tilde{V}$ and V, we see that $(K_1 \otimes K_2)\restriction_{\tilde{V}} = K$. Therefore, K is a positive definite kernel on V. ∎

4. Q-matrices. By a *graph* we mean a pair $G = (V, E)$, where V is a non-empty (finite or infinite) set and $E \subset \{\{x, y\} : x, y \in V,\, x \neq y\}$. An element of V is called a *vertex* and one in E an *edge*. We write $x \sim y$ if $\{x, y\} \in E$. A finite sequence of vertices $x_0, x_1, \ldots, x_n \in V$ is called a *walk* connecting $x, y \in V$ if

$$x = x_0 \sim x_1 \sim x_2 \sim \cdots \sim x_n = y.$$

In this case n is called the *length* of the walk. A graph is called *connected* if any two vertices $x, y \in V$, $x \neq y$, are connected by a walk. For a connected graph $G = (V, E)$ the *distance* between $x, y \in V$, $x \neq y$, is defined to be the shortest length of a walk connecting them, and is denoted by $\partial_G(x, y)$. By definition $\partial_G(x, x) = 0$ for all $x \in V$.

Throughout this paper a graph can be finite or infinite, but is always assumed to be connected. The *Q-matrix* of a graph $G = (V, E)$ is defined by

$$Q = Q(G; q) = [q^{\partial_G(x,y)}]_{x,y \in V}, \qquad q \in \mathbb{C}.$$

By definition the diagonal elements of $Q(G; q)$ are 1 for all q. We see easily that if G is non-trivial, i.e., $|V| \geq 2$, then $Q(G; q)$ can be pd only when $-1 \leq q \leq 1$. Accordingly, we set

$$\tilde{q}[G] = \{-1 \leq q \leq 1 : Q(G; q) \text{ is pd}\},$$
$$q[G] = \{-1 \leq q \leq 1 : Q(G; q) \text{ is spd}\}.$$

It is noted that $q[G] \subset \tilde{q}[G]$ and $\tilde{q}[G]$ is a closed subset of $[-1, 1]$.

Here are simple examples: For a complete graph K_n $(n \geq 2)$, we have

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

For a complete bipartite graph $K_{m,n}$ $(2 \leq m \leq n)$ we have

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

For the proofs and further examples, see [11, 15].

We close this section with the following simple fact.

Lemma 4.1. *Let $G = (V, E)$ be a graph and $H = (W, F)$ a subgraph, i.e., H is a graph with $W \subset V$ and $F \subset E$. Assume that both G and H are connected. If H is isometrically embedded in G, i.e.,*

$$\partial_H(x, y) = \partial_G(x, y), \qquad x, y \in W,$$

then $Q(H;q) = Q(G;q)\restriction_W$ *and*

$$q[G] \subset q[H], \qquad \tilde{q}[G] \subset \tilde{q}[H].$$

5. Graph products. To determine $q[G]$ and $\tilde{q}[G]$ is a difficult question in general. When a graph G is composed of two graphs G_1 and G_2 in some way, we may expect that the positivity of the Q-matrix of G would be inherited from that of the Q-matrices of G_1 and G_2. In this line the concept of detour join of two graphs is introduced in [15]. Our purpose here is to discuss four kinds of graph products: direct product (Cartesian product), star product, comb product, and free product.

In the following let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be connected graphs.

5.1. Direct product (Cartesian product). We set $V = V_1 \times V_2$ and

$$E = \left\{ \{(x_1, y_1), (x_2, y_2)\} : \begin{array}{l} \text{(i) } x_1 = x_2 \text{ and } \{y_1, y_2\} \in E_2, \\ \text{or (ii) } \{x_1, x_2\} \in E_1 \text{ and } y_1 = y_2 \end{array} \right\}.$$

Then $G = (V, E)$ is called the *direct product* or *Cartesian product* of G_1 and G_2, and is denoted by $G = G_1 \times G_2$.

LEMMA 5.1. *For two graphs* $G_1 = (V_1, E_1)$ *and* $G_2 = (V_2, E_2)$ *we have*

$$\partial_{G_1 \times G_2}((x_1, y_1), (x_2, y_2)) = \partial_{G_1}(x_1, x_2) + \partial_{G_2}(y_1, y_2)$$

for $x_1, x_2 \in V_1$ *and* $y_1, y_2 \in V_2$.

Proof. Straightforward and omitted. ∎

LEMMA 5.2. $Q(G_1 \times G_2\,; q) = Q(G_1; q) \otimes Q(G_2; q)$.

Proof. For simplicity we set $Q = Q(G_1 \times G_2; q)$, $Q_1 = Q(G_1; q)$ and $Q_2 = Q(G_2; q)$. By definition we have

$$Q((x_1, y_1), (x_2, y_2)) = q^{\partial_{G_1 \times G_2}((x_1, y_1), (x_2, y_2))},$$

$$Q_1(x_1, x_2) = q^{\partial_{G_1}(x_1, x_2)}, \quad Q_2(y_1, y_2) = q^{\partial_{G_2}(y_1, y_2)}.$$

Then by Lemma 5.1 we see that

$$Q((x_1, y_1), (x_2, y_2)) = Q_1(x_1, x_2) Q_2(y_1, y_2),$$

which means that $Q = Q_1 \otimes Q_2$. ∎

THEOREM 5.3. *For the direct product* $G_1 \times G_2$ *we have*

$$q[G_1 \times G_2] = q[G_1] \cap q[G_2], \qquad \tilde{q}[G_1 \times G_2] = \tilde{q}[G_1] \cap \tilde{q}[G_2].$$

Proof. For simplicity we set $Q = Q(G_1 \times G_2; q)$, $Q_1 = Q(G_1; q)$ and $Q_2 = Q(G_2; q)$. We only show the first relation, for the second is proved in a parallel manner.

Take $q \in q[G_1] \cap q[G_2]$. Since both Q_1 and Q_2 are pd, so is $Q_1 \otimes Q_2$ by Theorem 3.1. On the other hand, $Q = Q_1 \otimes Q_2$ by Lemma 5.2. Hence

$q \in q[G_1 \times G_2]$, so that $q[G_1] \cap q[G_2] \subset q[G_1 \times G_2]$. For the converse, we first note that, taking a cross section, G_1 and G_2 are isometrically embedded in $G = G_1 \times G_2$. Then applying Lemma 4.1, we see that $q[G_1 \times G_2] \subset q[G_1] \cap q[G_2]$. ■

5.2. Star product. Assume that two graphs G_1 and G_2 are equipped with distinguished vertices o_1 and o_2, respectively. The *star product* is defined to be a graph obtained by gluing G_1 and G_2 at the vertices o_1 and o_2. The star product is denoted by $G_1\,{}_{o_1}\!\star_{o_2} G_2$ or simply by $G_1 \star G_2$. For relevant discussion see [14].

LEMMA 5.4. *The star product $G = G_1 \star G_2$ is identified with the subgraph of the direct product $G_1 \times G_2$ induced (or spanned) by the vertices*

$$V = \{(o_1, y) : y \in V_2\} \cup \{(x, o_2) : x \in V_1\}.$$

Moreover, $G = G_1 \star G_2$ is isometrically embedded in $G_1 \times G_2$.

Proof. Straightforward by definition. ■

THEOREM 5.5. *For the star product $G_1 \star G_2$ we have*

$$q[G_1 \star G_2] = q[G_1] \cap q[G_2], \qquad \tilde{q}[G_1 \star G_2] = \tilde{q}[G_1] \cap \tilde{q}[G_2].$$

Proof. For simplicity we set $Q = Q(G_1 \star G_2; q)$, $Q_1 = Q(G_1; q)$ and $Q_2 = Q(G_2; q)$. We only show the first relation.

Combining Lemmas 5.4 and 4.1, we have

$$q[G_1 \star G_2] \supset q[G_1 \times G_2] = q[G_1] \cap q[G_2],$$

where Theorem 5.3 is also taken into account. On the other hand, G_1 and G_2 are isometrically embedded in $G_1 \star G_2$ in the obvious manner. It then follows from Theorem 4.1 that

$$q[G_1 \star G_2] \subset q[G_1] \cap q[G_2].$$

The assertion follows from the above two inclusion relations. ■

The positivity of the Haagerup states on a free group is a simple corollary. In fact, it is sufficient to consider a finite tree T. Since T is obtained by repeated application of the star product of K_2, appealing to Theorem 5.5 we obtain

$$q[T] = q[K_2] = (-1, 1), \qquad \tilde{q}[T] = \tilde{q}[K_2] = [-1, 1].$$

This argument, originally due to Bożejko [3], not only gave an alternative simple proof to Haagerup [9] but also broadened applications and indicated a further generalization.

5.3. Comb product. Assume that G_2 is equipped with a distinguished vertex $o_2 \in V_2$. We prepare $|V_1|$ copies of G_2. The *comb product* is defined to be the graph obtained by gluing each vertex of G_1 with a copy of G_2 at the vertex o_2. The comb product is denoted by $G_1 \rhd_{o_2} G_2$ or simply by

$G_1 \triangleright G_2$. By definition, $G_1 \triangleright G_2$ is identified with a subgraph (but not an induced subgraph) of $G_1 \times G_2$.

THEOREM 5.6. *For the comb product $G_1 \triangleright G_2$ we have*

$$q[G_1 \triangleright G_2] = q[G_1] \cap q[G_2], \qquad \tilde{q}[G_1 \triangleright G_2] = \tilde{q}[G_1] \cap \tilde{q}[G_2].$$

Proof. Since the comb product $G_1 \triangleright G_2$ is obtained by repeated application of star product, this a direct consequence of Theorem 5.5. ■

5.4. Free products. Given two graphs G_1 and G_2 with distinguished vertices, the free product $G_1 * G_2$ is defined. The construction shares a common spirit with free product groups. However, the formal definition is lengthy and omitted (see, e.g., [1, 8]).

THEOREM 5.7. *For the free product $G_1 * G_2$ we have*

$$q[G_1 * G_2] = q[G_1] \cap q[G_2], \qquad \tilde{q}[G_1 * G_2] = \tilde{q}[G_1] \cap \tilde{q}[G_2].$$

Proof. We may choose an increasing sequence $\{H_n\}$ of induced subgraphs of $G_1 * G_2$ such that (i) H_n is obtained by finitely many applications of star product of G_1 and G_2; (ii) H_n is isometrically embedded in $G_1 * G_2$; and (iii) $G_1 * G_2$ is the inductive limit of $\{H_n\}$. For example, H_n is taken to be the graph spanned by the vertices corresponding to the words of length $\leq n$. Then by Theorem 5.5 we obtain

$$q[G_1 * G_2] = q[H_n] = q[G_1] \cap q[G_2], \quad \tilde{q}[G_1 * G_2] = \tilde{q}[H_n] = \tilde{q}[G_1] \cap \tilde{q}[G_2],$$

as desired. ■

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