



# Distance matrices and quadratic embedding of graphs

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## Abstract

A connected graph is said to be of QE class if it admits a quadratic embedding in a Hilbert space, or equivalently, if the distance matrix is conditionally negative definite. Several criteria for a graph to be of QE class are derived from the point of view of graph operations. For a quantitative criterion the QE constant is introduced and concrete examples are shown with explicit calculation. If the distance matrix admits a constant row sum, the QE constant coincides with the second largest eigenvalue of the distance matrix. The QE constants are determined for all graphs on  $n$  vertices with  $n \leq 5$ , among which two are not of QE class.

*Keywords:* conditionally negative definite matrix, distance matrix, Euclidean distance matrix quadratic embedding, QE constant

Mathematics Subject Classification : 05C50, 05C12, 05C76

DOI: 10.5614/ejgta.2018.6.1.4

## 1. Introduction

Since Schoenberg [20, 21, 22] introduced essentially the concept of quadratic embedding of a metric space, many relevant works have appeared with wide applications often under the name of Euclidean distance geometry, see e.g., the excellent survey by Liberti *et al* [15] and references cited therein. In this line, discrete spaces have also attracted much attention from various aspects.

In this paper we focus on quadratic embedding of graphs, being motivated by two lines of researches. First, although less actively considered than the adjacency or Laplacian matrices, distance matrices are also interesting in characterization of graphs. Noteworthy characteristic properties of the distance matrices of trees are derived by Balaji–Bapat [2], see also Bapat [3, Chapter

Received: 22 August 2017, Revised: 9 January 2018, Accepted: 27 January 2018.

8]. More recently, Jaklič–Modić [11, 12, 13] determine some classes of graphs of QE class (in our terminology) and their explicit embeddings in Euclidean spaces. Second, the  $Q$ -matrix of a graph, the entrywise exponential of the distance matrix, has become important in relation to the  $q$ -deformation of spectral distributions of graphs, see e.g., Hora–Obata [9]. In this context it is fundamental to know whether the  $Q$ -matrix of a graph is positive definite or not. In fact, this property is closely related to that the graph admits a quadratic embedding, as is discussed by Haagerup [7] for a tree and by Božejko [5] for an elegant extension in terms of a Markov product. For further developments, see Obata [17, 18].

Now let  $G = (V, E)$  be a connected (finite or infinite) graph and denote by  $d(x, y)$  the graph distance between two vertices  $x, y \in V$ , i.e., the length of a shortest walk (or path) connecting  $x$  and  $y$ . A map  $\varphi$  from  $V$  into a Hilbert space  $\mathcal{H}$  is called a *quadratic embedding* of  $G$  if

$$\|\varphi(x) - \varphi(y)\|^2 = d(x, y), \quad x, y \in V, \quad (1)$$

where  $\|\cdot\|$  stands for the norm of  $\mathcal{H}$ . A graph  $G$  is said to be of *QE class* if it admits a quadratic embedding. A criterion for a graph  $G = (V, E)$  to be of QE class is given by a kind of spectral characteristic of the distance matrix  $D = [d(x, y)]_{x, y \in V}$ . In this paper we concentrate on the study of the *QE constant* of a graph  $G$  defined by

$$\text{QEC}(G) = \sup\{\langle f, Df \rangle; f \in C_0(V), \langle f, f \rangle = 1, \langle \mathbf{1}, f \rangle = 0\}, \quad (2)$$

for notations see Section 2. By definition the distance matrix  $D$  is conditionally negative definite if and only if  $\text{QEC}(G) \leq 0$ . The crucial fact due to Schoenberg [20, 21] (also Young–Householder [23] for a finite case) says that a graph  $G$  admits a quadratic embedding if and only if  $D$  is conditionally negative definite. We thus have a quantitative criterion: a graph  $G$  is of QE class if and only if  $\text{QEC}(G) \leq 0$ . The main purpose of this paper is to derive several criteria for a graph to be of QE class, and provide concrete examples with explicit QE constants. We consider the QE constant itself as an interesting spectral characteristic of a graph.

This paper is organized as follows: In Section 2, after preparation of basic notations and notions, we examine paths  $P_n$ , cycles  $C_n$ , complete graphs  $K_n$ , complete bipartite graphs  $K_{m,n}$ , a tri-partite graphs  $K_{1,1,n}$  and so on as first examples.

In Section 3 we discuss graph operations preserving the property of being of QE class, in particular, isometric embedding of a subgraph, the Cartesian product, the star product, and deletion of edges. It is noteworthy that  $\text{QEC}(G_1 \times G_2) = 0$  holds whenever both  $G_1$  and  $G_2$  are graphs of QE class on two or more vertices (Theorem 3.3). The star product preserves the property of being QE class (Theorem 3.5). Deleting edges from the complete graphs, we construct graphs of QE class and of non-QE class.

In Section 4 we provide two methods of calculating the QE constants. As is anticipated from the definition (2), the method of Lagrange multipliers gives rise to a concise formula, but not very practical (Proposition 4.2). The second method uses eigenvalues of the distance matrix. It is shown that  $\text{QEC}(G)$  coincides with the second largest eigenvalue of  $D$  if the distance matrix admits a constant row sum (Theorem 4.7). The second method is restrictive but still covers a wide class of graphs.

In Section 5 we examine all graphs on  $n$  vertices with  $2 \leq n \leq 5$  together with their QE constants. As a result, there are two graphs which are not of QE class. It seems that these two

graphs are well-known among experts, but not easily found in literatures. The full list will be useful in the further study of graph operations and non-QE graphs.

## 2. Graphs of QE class

### 2.1. Notations

For a non-empty set  $X$  let  $C(X)$  denote the space of  $\mathbb{R}$ -valued functions on  $X$ , and  $C_0(X)$  the subspace of ones with finite supports. Obviously,  $C_0(X) = C(X)$  if  $X$  is finite. The canonical inner product and norm on  $C_0(X)$  are defined by

$$\langle f, g \rangle = \sum_{x \in X} f(x) g(x), \quad \|f\| = \sqrt{\langle f, f \rangle}, \quad f, g \in C_0(X),$$

respectively. Let  $\mathbf{1} \in C(X)$  be the constant function defined by  $\mathbf{1}(x) = 1$  for all  $x \in X$ . Overusing the notation, we write

$$\langle \mathbf{1}, f \rangle = \sum_{x \in X} f(x), \quad f \in C_0(X).$$

A  $\mathbb{R}$ -valued function  $K : X \times X \rightarrow \mathbb{R}$ , i.e.,  $K \in C(X \times X)$ , is called a *kernel* on  $X$  or a *matrix* with index set  $X \times X$ , and we write

$$K = [K(x, y)] = [K(x, y)]_{x, y \in X}, \quad (K)_{xy} = K(x, y).$$

In accordance with usual matrix multiplication, for  $K \in C(X \times X)$  and  $f \in C_0(X)$  we define

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

Then  $Kf \in C(X)$  but not necessarily  $Kf \in C_0(X)$ . Overusing the notation again, we write

$$\langle f, Kg \rangle = \sum_{x, y} K(x, y)f(x)g(y), \quad f, g \in C_0(X).$$

The canonical basis of  $C_0(X)$  is denoted by  $\{e_x; x \in X\}$ , where  $e_x(y) = \delta_{xy}$  (Kronecker symbol). Obviously,  $\langle e_x, e_y \rangle = \delta_{xy}$ . Note the obvious relation:

$$\langle e_x, Ke_y \rangle = K(x, y), \quad x, y \in X.$$

The *transposed matrix* is defined by  $K^T(x, y) = K(y, x)$ . We then have

$$\langle f, Kg \rangle = \langle K^T f, g \rangle, \quad f, g \in C_0(X).$$

A matrix  $K$  is called *symmetric* if  $K^T = K$ .

2.2. *Conditionally negative definite matrices and quadratic embedding of a metric space*

A symmetric matrix  $K = [K(x, y)]$  with index set  $X \times X$  is called *conditionally negative definite* if

$$\langle f, Kf \rangle = \sum_{x, y \in X} K(x, y) f(x) f(y) \leq 0$$

for all  $f \in C_0(X)$  with  $\langle \mathbf{1}, f \rangle = 0$ .

Let  $(X, d)$  be a metric space. A map  $\varphi$  from  $X$  into a Hilbert space  $\mathcal{H}$  is called a *quadratic embedding* of  $(X, d)$  if

$$\|\varphi(x) - \varphi(y)\|^2 = d(x, y), \quad x, y \in X,$$

where  $\|\cdot\|$  is the norm of the Hilbert space  $\mathcal{H}$ . The following result is due to Schoenberg [21], for relevant results see also Hayden–Reams–Wells [8], Józziak [14], Young–Householder [23].

**Theorem 2.1.** *For a metric space  $(X, d)$  the following two conditions are equivalent:*

- (i) *the metric space  $(X, d)$  admits a quadratic embedding;*
- (ii) *the distance matrix  $D = [d(x, y)]_{x, y \in X}$  is conditionally negative definite.*

*Remark 2.2.* A symmetric matrix  $K$  satisfying  $K(x, x) = 0$  for all  $x \in X$  is called a *Schoenberg kernel*. A finite symmetric matrix  $K$  is called a *Euclidean distance matrix* if there is a map  $\varphi$  from  $X$  into a Euclidean space such that  $K(x, y) = \|\varphi(x) - \varphi(y)\|^2$  for all  $x, y \in X$ .

2.3. *QE constants of graphs*

A *graph* is a pair  $G = (V, E)$ , where  $V$  is a non-empty set of vertices and  $E$  a set of edges, i.e., a subset of  $\{\{x, y\}; x, y \in V, x \neq y\}$ . If  $\{x, y\} \in E$ , we write  $x \sim y$  for simplicity. A finite sequence of vertices  $x_0, x_1, \dots, x_m \in V$  is called an *m-step walk* if  $x_0 \sim x_1 \sim \dots \sim x_m$ . In this case we say that  $x_0$  and  $x_m$  are connected by a walk of length  $m$ . A graph is called *connected* if any pair of vertices are connected by a walk. A graph is called *finite* if  $V$  is a finite set. Throughout this paper by a graph we always mean a (finite or infinite) connected graph.

For  $x, y \in V$  with  $x \neq y$  let  $d(x, y)$  denote the length of a shortest walk (or path) connecting  $x$  and  $y$ . By definition we set  $d(x, x) = 0$ . Then  $d(x, y)$  becomes a metric on  $V$ , which we call the *graph distance*. A graph  $G = (V, E)$  is called of *QE class* if the metric space  $(V, d)$  admits a quadratic embedding, i.e., there exist a Hilbert space  $\mathcal{H}$  and a map  $\varphi : V \rightarrow \mathcal{H}$  such that

$$\|\varphi(x) - \varphi(y)\|^2 = d(x, y), \quad x, y \in V.$$

Such a map  $\varphi$  is called a *quadratic embedding* of  $G$ .

Let  $D = [d(x, y)]_{x, y \in V}$  be the distance matrix of a graph  $G = (V, E)$ . The *QE constant* of a graph  $G$  is defined by

$$\text{QEC}(G) = \sup\{\langle f, Df \rangle; f \in C_0(V), \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\}. \tag{3}$$

Obviously,  $\text{QEC}(G)$  is characterized as the infimum among constants  $C$  satisfying

$$\langle f, Df \rangle \leq C\|f\|^2 \quad \text{for all } f \in C_0(V) \text{ with } \langle \mathbf{1}, f \rangle = 0.$$

By definition  $D$  is conditionally negative definite if and only if  $\text{QEC}(G) \leq 0$ . Then, combining Theorem 2.1, we come to the following

**Theorem 2.3.** Let  $G = (V, E)$  be a graph with distance matrix  $D = [d(x, y)]$ . Then the following conditions are equivalent:

- (i)  $G$  is of QE class;
- (ii)  $D$  is conditionally negative definite;
- (iii)  $\text{QEC}(G) \leq 0$ .

*Remark 2.4.* If  $G$  is a finite graph, say  $V = \{1, 2, \dots, n\}$ , then through the natural identification of  $C(V)$  with  $\mathbb{R}^n$  the domain

$$\{f \in \mathbb{R}^n; \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\}$$

is homeomorphic to a sphere of  $n - 2$  dimension. Therefore,  $\text{QEC}(G)$  is attained by some  $f \in \mathbb{R}^n$  with  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , that is,

$$\text{QEC}(G) = \max\{\langle f, Df \rangle; f \in C(V), \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\}. \tag{4}$$

#### 2.4. First examples of graphs of QE class

**Theorem 2.5** (Jaklič–Modić [11]). For any  $n \geq 1$  the path  $P_n$  on  $n$  vertices is of QE class.

**Theorem 2.6.** For any  $n \geq 1$  the complete graph  $K_n$  on  $n$  vertices is of QE class.

In fact, a path along the mutually vertical edges of a hypercube gives rise to a quadratic embedding of  $P_n$  into  $\mathbb{R}^{n-1}$ . Similarly, a natural realization of  $K_n$  as a regular polytope in  $\mathbb{R}^{n-1}$  is a quadratic embedding.

The QE constant of  $K_n$  is obtained easily. Taking  $V = \{1, 2, \dots, n\}$ , we see that all entries of  $D$  are 1 except the zero diagonals. Then for  $f = [x_1 \cdots x_n]^T \in \mathbb{R}^n$  we have

$$\langle f, Df \rangle = \sum_{i \neq j} x_i x_j = \sum_{i,j=1}^n x_i x_j - \sum_{i=1}^n x_i^2 = \langle \mathbf{1}, f \rangle^2 - \|f\|^2.$$

Obviously,  $\langle f, Df \rangle \leq 0$  whenever  $\langle \mathbf{1}, f \rangle = 0$ . Moreover, for  $n \geq 2$  we have

$$\text{QEC}(K_n) = \max\{\langle f, Df \rangle; f \in C(V), \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\} = -1.$$

Note that  $\text{QEC}(K_1) = 0$  by definition.

**Theorem 2.7** (Jaklič–Modić [12]). For any  $n \geq 3$  the cycle  $C_n$  is of QE class.

Calculation of  $\text{QEC}(C_n)$  is postponed, see Example 4.9.

**Theorem 2.8.** Let  $1 \leq m \leq n$ . The complete bipartite graph  $K_{m,n}$  is of QE class if and only if

- (i)  $m = 1$  and  $n \geq 1$ , that is,  $K_{1,n}$  is a star; or
- (ii)  $m = n = 2$ , that is,  $K_{2,2} \cong C_4$  is a cycle on 4 vertices.

*Proof.* The distance matrix is written in the form:

$$D = \begin{bmatrix} A & J \\ J^T & B \end{bmatrix},$$

where  $A$  is an  $m \times m$  matrix with off-diagonal entries being all 2 and diagonal ones all 0,  $B$  is an  $n \times n$  matrix of the same type, and  $J$  is an  $m \times n$  matrix with entries being all 1. For  $f = [x_1 \cdots x_m y_1 \cdots y_n]^T \in \mathbb{R}^{m+n}$  we have

$$\begin{aligned} \langle f, Df \rangle &= 2 \sum_{1 \leq i \neq j \leq m} x_i x_j + 2 \sum_{i=1}^m \sum_{j=1}^n x_i y_j + 2 \sum_{1 \leq i \neq j \leq n} y_i y_j \\ &= 2 \left( \sum_{i,j=1}^m x_i x_j - \sum_{i=1}^m x_i^2 \right) + 2 \sum_{i=1}^m \sum_{j=1}^n x_i y_j + 2 \left( \sum_{i,j=1}^n y_i y_j - \sum_{j=1}^n y_j^2 \right) \\ &= -2 \left( \sum_{i=1}^m x_i^2 + \sum_{j=1}^n y_j^2 \right) + 2 \left( \sum_{i,j=1}^m x_i x_j + \sum_{i=1}^m \sum_{j=1}^n x_i y_j + \sum_{i,j=1}^n y_i y_j \right). \end{aligned} \quad (5)$$

It is sufficient to find the maximum of  $\langle f, Df \rangle$ , where  $f \in \mathbb{R}^{m+n}$  runs over the domain determined by

$$\|f\|^2 = \langle f, f \rangle = \sum_{i=1}^m x_i^2 + \sum_{j=1}^n y_j^2 = 1, \quad \langle \mathbf{1}, f \rangle = \sum_{i=1}^m x_i + \sum_{j=1}^n y_j = 0. \quad (6)$$

The above conditions being taken into account, (5) admits a simpler expression:

$$\langle f, Df \rangle = -2 + 2 \left( \sum_{i=1}^m x_i \right)^2.$$

The maximum of  $\langle f, Df \rangle$  subject to (6) is computed by elementary calculus (see Appendix No. 1) and we come to

$$\text{QEC}(K_{m,n}) = -2 + \frac{2mn}{m+n} = \frac{2}{m+n} \{(m-1)(n-1) - 1\},$$

from which the assertion follows immediately. □

**Theorem 2.9.** *Let  $n \geq 1$ . A tri-partite graph  $K_{1,1,n}$  is of QE class if and only if  $1 \leq n \leq 4$ .*

*Proof.* Let  $V = \{1, 2, \dots, n, n+1, n+2\}$  and assume that the three components are given by  $\{1, 2, \dots, n\}$ ,  $\{n+1\}$  and  $\{n+2\}$ . For  $f = [x_1 \cdots x_n x_{n+1} x_{n+2}]^T \in \mathbb{R}^{n+2}$ , under the conditions  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  we have

$$\langle f, Df \rangle = -\|f\|^2 + \sum_{1 \leq i < j \leq n} 2x_i x_j,$$

of which the maximum subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  is the QE constant. By elementary calculus (see Appendix No. 3) we obtain

$$\text{QEC}(K_{1,1,n}) = -1 + \frac{(n-1)\{(n+2) - n\}}{n+2} = \frac{n-4}{n+2},$$

which proves the assertion. □

*Remark 2.10.* The tri-partite graph  $K_{1,1,n}$  is also called the  $n$ -fold edge-amalgamation of  $K_3$ .

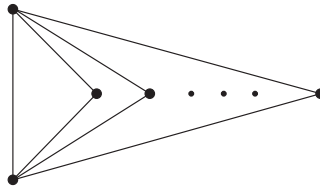


Figure 1.  $K_{1,1,n}$ :  $n$ -fold edge amalgamation of  $K_3$

### 3. Graph operations preserving QE class

#### 3.1. Subgraphs

**Theorem 3.1.** Let  $G = (V, E)$  be a subgraph of  $\tilde{G} = (\tilde{V}, \tilde{E})$ . Let  $d$  and  $\tilde{d}$  be the graph distances of  $G$  and  $\tilde{G}$ , respectively. If  $d(x, y) = \tilde{d}(x, y)$  for all  $x, y \in V$ , i.e.,  $G$  is isometrically embedded in  $\tilde{G}$ , then we have

$$\text{QEC}(G) \leq \text{QEC}(\tilde{G}).$$

In particular, if  $\tilde{G}$  is of QE class, so is  $G$ .

*Proof.* Let  $\tilde{D}$  and  $D$  be the distance matrices of  $\tilde{G}$  and  $G$ , respectively. Then  $\tilde{D}$  admits an expression in the form of block matrices:

$$\tilde{D} = \begin{bmatrix} D & C \\ C^T & B \end{bmatrix}.$$

By definition of  $\text{QEC}(G)$ , for any  $\epsilon > 0$  there exists an  $f \in C_0(V)$  with  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  such that  $\langle f, Df \rangle \geq \text{QEC}(G) - \epsilon$ . Define  $\tilde{f} \in C_0(\tilde{V})$  by  $\tilde{f}(x) = f(x)$  for  $x \in V$  and  $= 0$  otherwise. Then, we have  $\|\tilde{f}\| = 1$ ,  $\langle \mathbf{1}, \tilde{f} \rangle = 0$  and

$$\langle \tilde{f}, \tilde{D}\tilde{f} \rangle = \left\langle \begin{bmatrix} f \\ 0 \end{bmatrix}, \begin{bmatrix} D & C \\ C^T & B \end{bmatrix} \begin{bmatrix} f \\ 0 \end{bmatrix} \right\rangle = \langle f, Df \rangle \geq \text{QEC}(G) - \epsilon.$$

Hence  $\text{QEC}(\tilde{G}) \geq \text{QEC}(G) - \epsilon$ . Since  $\epsilon > 0$  is arbitrary, we have  $\text{QEC}(\tilde{G}) \geq \text{QEC}(G)$ . □

Theorem 3.1 is useful for constructing a graph of not QE class from a smaller one. For example,

**Proposition 3.2.** Let  $G = (V, E)$  be a graph with  $\text{diam}(G) \leq 2$ . Let  $\tilde{G} = (\tilde{V}, \tilde{E})$  be a graph obtained by adding a vertex to  $G$  with one or more edges. If  $G$  is not of QE class, either is not  $\tilde{G}$ .

### 3.2. Cartesian product

For two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  the Cartesian product  $G_1 \times G_2$  is defined to be a graph on  $V_1 \times V_2$  with the adjacency relation:

$$(x_1, y_1) \sim (x_2, y_2) \iff \text{(i) } \begin{matrix} x_1 \sim x_2, \\ y_1 = y_2 \end{matrix} \quad \text{or} \quad \text{(ii) } \begin{matrix} x_1 = x_2, \\ y_1 \sim y_2. \end{matrix}$$

**Theorem 3.3.** *If both  $G_1$  and  $G_2$  are of QE class, so is the Cartesian product  $G_1 \times G_2$ . Moreover,  $\text{QEC}(G_1 \times G_2) = 0$  whenever  $|V_1| \geq 2$  and  $|V_2| \geq 2$ .*

*Proof.* For  $i = 1, 2$  let  $\alpha_i : V_i \rightarrow \mathcal{H}_i$  be a quadratic embedding. Define a map  $\beta : V_1 \times V_2 \rightarrow \mathcal{H}_1 \oplus \mathcal{H}_2$  by

$$\beta(x, y) = \alpha_1(x) \oplus \alpha_2(y), \quad x \in V_1, \quad y \in V_2.$$

We then see that

$$\begin{aligned} \|\beta(x_1, y_1) - \beta(x_2, y_2)\|^2 &= \|\alpha_1(x_1) \oplus \alpha_2(y_1) - \alpha_1(x_2) \oplus \alpha_2(y_2)\|^2 \\ &= \|(\alpha_1(x_1) - \alpha_1(x_2)) \oplus (\alpha_2(y_1) - \alpha_2(y_2))\|^2 \\ &= \|\alpha_1(x_1) - \alpha_1(x_2)\|^2 + \|\alpha_2(y_1) - \alpha_2(y_2)\|^2. \end{aligned} \tag{7}$$

Let  $d_1$  and  $d_2$  be the graph distances of  $G_1$  and  $G_2$ , respectively. Since  $\alpha_1$  and  $\alpha_2$  are quadratic embeddings, (7) becomes

$$\|\beta(x_1, y_1) - \beta(x_2, y_2)\|^2 = d_1(x_1, x_2) + d_2(y_1, y_2). \tag{8}$$

On the other hand, the graph distance  $d$  of  $G = G_1 \times G_2$  satisfies

$$d((x_1, y_1), (x_2, y_2)) = d_1(x_1, x_2) + d_2(y_1, y_2).$$

Hence (8) means that  $\beta$  is a quadratic embedding of  $G$  into  $\mathcal{H}_1 \oplus \mathcal{H}_2$ . Therefore  $G$  is of QE class and  $\text{QEC}(G) \leq 0$ .

In order to infer that  $\text{QEC}(G) = 0$  it is sufficient to show that  $\langle f, Df \rangle = 0$  holds for some  $f \in C_0(V)$  satisfying  $\langle \mathbf{1}, f \rangle = 0$  and  $f \neq 0$ . In fact, for  $i = 1, 2$  choosing  $g_i \in C_0(V_i)$  such that  $\langle \mathbf{1}, g_i \rangle = 0$  and  $g_i \neq 0$  (this is possible whenever  $|V_i| \geq 2$ ), we see easily that  $f(x, y) = g_1(x)g_2(y)$  possesses the desired properties.  $\square$

**Example 3.4.** Since  $C_4 \cong K_2 \times K_2$  we have  $\text{QEC}(C_4) = 0$  by Theorem 3.3. That  $C_4$  is of QE class follows also from Theorems 2.7 and 2.8.

### 3.3. Star product

Suppose that two graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  are given with distinguished vertices  $o_1 \in V_1$  and  $o_2 \in V_2$ , respectively. The graph obtained by gluing vertices  $o_1$  and  $o_2$  is called the *star product* or the vertex amalgamation, and is denoted by  $G_1 \star G_2$ . It is convenient to write the vertex set of  $G_1 \star G_2$  as

$$V = (V_1 \setminus \{o_1\}) \cup (V_2 \setminus \{o_2\}) \cup \{o\},$$



where  $o$  corresponds to the glued vertices  $o_1$  and  $o_2$ . Let  $d_i$  denote the graph distance of  $G_i$  for  $i = 1, 2$ , and  $d$  the graph distance of  $G_1 \star G_2$ . Then we have

$$d(x, y) = \begin{cases} d_1(x, y), & \text{if } x, y \in V_1, \\ d_1(x, o) + d_2(o, y), & \text{if } x \in V_1 \text{ and } y \in V_2, \\ d_2(x, o) + d_1(o, y), & \text{if } x \in V_2 \text{ and } y \in V_1, \\ d_2(x, y), & \text{if } x, y \in V_2. \end{cases}$$

**Theorem 3.5.** *If both  $G_1$  and  $G_2$  are of QE class, so is the star product  $G_1 \star G_2$ .*

*Proof.* For  $i = 1, 2$  let  $\alpha_i : V_i \rightarrow \mathcal{H}_i$  be a quadratic embedding. We may assume that  $\alpha_i(o_i) = 0$ . Define a map  $\beta : V \rightarrow \mathcal{H}_1 \oplus \mathcal{H}_2$  by

$$\beta(x) = \begin{cases} \alpha_1(x) \oplus 0, & \text{if } x \in V_1; \\ 0 \oplus \alpha_2(x), & \text{if } x \in V_2. \end{cases}$$

Note that  $\beta(o) = 0 \oplus 0$  follows from  $\alpha_1(o_1) = \alpha_2(o_2) = 0$ . We will show that

$$\|\beta(x) - \beta(y)\|^2 = d(x, y), \quad x, y \in V. \tag{9}$$

In fact, if  $x, y \in V_1$ , we have

$$\|\beta(x) - \beta(y)\|^2 = \|\alpha_1(x) - \alpha_1(y)\|^2 = d_1(x, y) = d(x, y).$$

Similarly, (9) is verified for  $x, y \in V_2$ . For  $x \in V_1$  and  $y \in V_2$  we have

$$\begin{aligned} \|\beta(x) - \beta(y)\|^2 &= \|\alpha_1(x) \oplus 0 - 0 \oplus \alpha_2(y)\|^2 = \|\alpha_1(x)\|^2 + \|\alpha_2(y)\|^2 \\ &= \|\alpha_1(x) - \alpha_1(o_1)\|^2 + \|\alpha_2(y) - \alpha_2(o_2)\|^2 \\ &= d(x, o_1) + d(y, o_2) = d(x, y). \end{aligned}$$

Thus,  $\beta$  is a quadratic embedding and  $G_1 \star G_2$  is of QE class. □

A star product of  $G$  and  $K_2 \cong P_2$  is called a *segment concatenation* of  $G$ . Since  $K_2$  is of QE class, we have the following

**Corollary 3.6.** *If  $G$  is a graph of QE class, so is any segment concatenation of  $G$ .*

**Corollary 3.7.** *Any tree is of QE class.*

*Remark 3.8.* In some literatures, the *star product* of  $G_1$  and  $G_2$  is defined to be a graph on  $V_1 \times V_2$  equipped with the adjacency relation defined by

$$(x_1, y_1) \sim (x_2, y_2) \iff \text{(i) } \begin{matrix} x_1 \sim x_2, \\ y_1 = y_2 = o_2, \end{matrix} \quad \text{or} \quad \text{(ii) } \begin{matrix} x_1 = x_2 = o_1, \\ y_1 \sim y_2, \end{matrix}$$

see e.g., Obata [19]. According to this definition the star product contains many isolated vertices. The connected component containing  $(o_1, o_2)$  coincides with  $G_1 \star G_2$  defined at the beginning of this subsection.

3.4. Deleting edges from complete graphs

For a graph  $G = (V, E)$  and a subset  $E_0 \subset E$  we define  $G \setminus E_0 = (V, E \setminus E_0)$ , which is the graph obtained from the original graph  $G$  by deleting edges in  $E_0$ . We consider graphs obtained from the complete graph  $K_n$  by deleting edges. The vertex set of  $K_n$  is taken to be  $V = \{1, 2, \dots, n\}$  and  $f \in C(V)$  is identified with a column vector  $[x_1 \cdots x_n]^T \in \mathbb{R}^n$ .

We start with the case of deleting edges which are mutually disjoint.

**Theorem 3.9.** *Let  $r \geq 1$  and  $2r \leq n$ . The graph obtained from the complete graph  $K_n$  by deleting  $r$  mutually disjoint edges, denoted by  $K_n \setminus \{e_1, \dots, e_r\}$ , is of QE class and*

$$\begin{aligned} \text{QEC}(K_n \setminus \{e_1\}) &= -\frac{2}{n}, \\ \text{QEC}(K_n \setminus \{e_1, \dots, e_r\}) &= 0, \quad r \geq 2. \end{aligned}$$

*Proof.* Without loss of generality we may assume that  $e_1 = \{1, 2\}$ ,  $e_2 = \{3, 4\}$ ,  $\dots$ ,  $e_r = \{2r - 1, 2r\}$ . Then, under the conditions  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , we have

$$\langle f, Df \rangle = -\|f\|^2 + 2x_1x_2 + 2x_3x_4 + \dots + 2x_{2r-1}x_{2r}.$$

of which the maximum subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  is the QE constant of  $K_n \setminus \{e_1, \dots, e_r\}$ . First for  $r = 1$  an elementary argument (see Appendix No. 3) shows that

$$\max \{2x_1x_2; \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\} = \frac{n - 2}{n}$$

and hence,

$$\text{QEC}(K_n \setminus \{e_1\}) = -1 + \frac{n - 2}{n} = -\frac{2}{n}.$$

For  $r \geq 2$  we apply Appendix No. 4 to obtain

$$\text{QEC}(K_n \setminus \{e_1, \dots, e_r\}) = -1 + 1 = 0.$$

In particular,  $K_n \setminus \{e_1, \dots, e_r\}$  is of QE class. □

**Example 3.10.** Note that  $C_4 \cong K_4 \setminus \{e_1, e_2\}$ , where  $e_1$  and  $e_2$  are mutually disjoint edges. Then  $\text{QEC}(C_4) = 0$  follows also from Theorem 3.9.

Let us consider the case of deleting two edges  $e_1$  and  $e_2$  which are connected. We write  $K_n \setminus P_3 = K_n \setminus \{e_1, e_2\}$  for convenience.

**Theorem 3.11.** *Let  $n \geq 4$ . We have*

$$\text{QEC}(K_n \setminus P_3) = \frac{n - 10}{n + 2 + \sqrt{2(n - 1)(n - 2)}}.$$

*In particular,  $K_n \setminus P_3$  is of QE class if and only if  $4 \leq n \leq 10$ .*

*Proof.* Without loss of generality we may assume that  $e_1 = \{1, 2\}$  and  $e_2 = \{1, 3\}$ . Then, under the conditions  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , we have

$$\langle f, Df \rangle = -\|f\|^2 + 2x_1x_2 + 2x_1x_3.$$

With the help of Appendix No. 5 we come to

$$\text{QEC}(K_n \setminus P_3) = -1 + \frac{-2 + \sqrt{2(n-1)(n-2)}}{n},$$

from which the assertion follows immediately. □

Finally, we consider the case of deleting edges of a clique, i.e., a subgraph isomorphic to a complete graph. To be precise, for  $2 \leq r < n$  we denote by  $K_n \setminus K_r$  the graph obtained from  $K_n$  by deleting  $r(r-1)/2$  edges which constitute a complete graph on  $r$  vertices. Note that no vertex is deleted.

**Theorem 3.12.** *For  $2 \leq r < n$  we have*

$$\text{QEC}(K_n \setminus K_r) = r - 2 - \frac{r(r-1)}{n}.$$

*In particular,  $K_n \setminus K_r$  is of QE class if and only if one of the following four cases occurs:*

- (i)  $r = 2$  and  $n \geq 3$ ;
- (ii)  $r = 3$  and  $n = 4, 5, 6$ ;
- (iii)  $r = 4$  and  $n = 5, 6$ ;
- (iv)  $r \geq 5$  and  $n = r + 1$ .

*Proof.* Let  $\{1, 2, \dots, r\}$  be the set of vertices of  $K_r$ . Then, under the conditions  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , we have

$$\langle f, Df \rangle = -\|f\|^2 + \sum_{1 \leq i < j \leq r} 2x_i x_j,$$

of which the maximum subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  is the QE constant of  $K_n \setminus K_r$ . With the help of Appendix No. 3 we come to

$$\text{QEC}(K_n \setminus K_r) = -1 + \frac{(r-1)(n-r)}{n} = r - 2 - \frac{r(r-1)}{n},$$

as desired. The rest of the assertion follows by a simple algebra. □

*Remark 3.13.* Since the tri-partite graph  $K_{1,1,n}$  is obtained as  $K_{n+2} \setminus K_n$ , Theorem 2.9 is a consequence of Theorem 3.12.

#### 4. Calculating QE constants of finite graphs

##### 4.1. Method of Lagrange multipliers

Let  $G = (V, E)$  be a graph on  $V = \{1, 2, \dots, n\}$  with  $n \geq 3$ , and  $D$  the distance matrix of  $G$  as usual. We identify  $f \in C(V)$  with a column vector  $[x_1 \dots x_n]^T \in \mathbb{R}^n$ . By definition the QE constant is the maximum of  $\langle f, Df \rangle$  subject to

$$\|f\|^2 = \langle f, f \rangle = \sum_{i=1}^n x_i^2 = 1, \tag{10}$$

$$\langle \mathbf{1}, f \rangle = \sum_{i=1}^n x_i = 0. \tag{11}$$

We set

$$F(f, \lambda, \mu) = \langle f, Df \rangle - \lambda(\langle f, f \rangle - 1) - \mu\langle \mathbf{1}, f \rangle. \tag{12}$$

By differentiation we obtain

$$\frac{\partial F}{\partial x_i} = 2\langle e_i, Df \rangle - 2\lambda\langle e_i, f \rangle - \mu\langle \mathbf{1}, e_i \rangle = \langle e_i, 2(D - \lambda)f - \mu\mathbf{1} \rangle,$$

where  $\{e_i\}$  is the canonical basis of  $\mathbb{R}^n$ . Hence  $\partial F/\partial x_i = 0$  for all  $1 \leq i \leq n$  is equivalent to  $2(D - \lambda)f - \mu\mathbf{1} = 0$ , that is,

$$(D - \lambda)f = \frac{\mu}{2}\mathbf{1}. \tag{13}$$

Let  $\mathcal{S}(D)$  be the set of  $(f = [x_i], \lambda, \mu)$  satisfying (10), (11) and (13).

Since relations (10) and (11) define a sphere of  $n - 2$  dimension, which is smooth and compact, the maximum of  $\langle f, Df \rangle$  is attained at a certain  $f$  appearing in  $\mathcal{S}(D)$ . On the other hand, for  $(f, \lambda, \mu) \in \mathcal{S}(D)$  we have

$$\langle f, Df \rangle = \langle f, \lambda f + \frac{\mu}{2}\mathbf{1} \rangle = \lambda\langle f, f \rangle + \frac{\mu}{2}\langle f, \mathbf{1} \rangle = \lambda. \tag{14}$$

Consequently, the maximum to be found coincides with the maximum of  $\lambda$  appearing in  $\mathcal{S}(D)$ .

The above argument is summarized in the following

**Proposition 4.1.** *Let  $D$  be the distance matrix of a graph  $G$  on  $n$  vertices with  $n \geq 3$ . Let  $\mathcal{S}(D)$  be the set of  $(f = [x_i], \lambda, \mu)$  satisfying (10), (11) and (13). Then  $\text{QEC}(G)$  coincides with the maximum of  $\lambda$  appearing in  $\mathcal{S}(D)$ .*

We go back to equation (13). Suppose first that  $\lambda \notin \text{ev}(D)$ , or equivalently  $\det(D - \lambda) \neq 0$ . Then from (13) we obtain

$$f = \frac{\mu}{2}(D - \lambda)^{-1}\mathbf{1}. \tag{15}$$

Moreover, (10) and (11) become

$$\frac{\mu^2}{4}\|(D - \lambda)^{-1}\mathbf{1}\|^2 = 1, \tag{16}$$

$$\frac{\mu}{2}\langle \mathbf{1}, (D - \lambda)^{-1}\mathbf{1} \rangle = 0, \tag{17}$$

respectively. Note that  $\mu \neq 0$  by (16). After solving the equation

$$\langle \mathbf{1}, (D - \lambda)^{-1} \mathbf{1} \rangle = 0, \tag{18}$$

we decide  $\mu$  by (16) and then  $f$  by (15). Recall that

$$(D - \lambda)^{-1} = \frac{1}{\det(D - \lambda)} [p_{ij}(\lambda)], \tag{19}$$

where  $p_{ij}(\lambda)$  is the  $(j, i)$ -cofactor of  $D - \lambda$ , i.e.,  $(-1)^{i+j}$  times the determinant of the submatrix obtained by deleting  $j$ th row and  $i$ th column of  $D - \lambda$ . We then see that equation (18) is equivalent to an algebraic equation:

$$P(\lambda) = 0,$$

where

$$P(\lambda) = \sum_{i,j=1}^n p_{ij}(\lambda).$$

Since  $p_{ij}(\lambda)$  is a polynomial of degree at most  $n - 1$ , so is  $P(\lambda)$ . Taking in mind that the zeros of  $P(\lambda)$  may contain an eigenvalue of  $D$ , we set

$$\Lambda_1(D) = \{\lambda \in \mathbb{R}; P(\lambda) = 0\} \setminus \text{ev}(D).$$

Then, for each  $\lambda \in \Lambda_1(D)$  we may construct a solution  $(f, \lambda, \mu) \in \mathcal{S}(D)$ .

Let  $\Lambda_2(D)$  denote the set of eigenvalues  $\lambda \in \text{ev}(D)$  which generate solutions  $(f, \lambda, \mu) \in \mathcal{S}(D)$ . Then Proposition 4.1 may be rephrased as follows.

**Proposition 4.2.** *Let  $D$  be the distance matrix of a graph  $G$  on  $n$  vertices with  $n \geq 3$ . Let  $\Lambda_1(D)$  and  $\Lambda_2(D)$  be as above. Then,*

$$\text{QEC}(G) = \max \Lambda_1(D) \cup \Lambda_2(D). \tag{20}$$

Formula (20) looks concise, however, involves many routine calculations and further improvement is necessary for application. The situation is suggested by the examples below.

**Example 4.3.** Consider  $K_3 \star K_2$  with distance matrix

$$D = \begin{bmatrix} 0 & 1 & 2 & 2 \\ 1 & 0 & 1 & 1 \\ 2 & 1 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{bmatrix}.$$

First we have

$$\det(\lambda - D) = (\lambda + 1)(\lambda^3 - \lambda^2 - 11\lambda - 7),$$

from which we see that  $D$  has four distinct real eigenvalues. A direct calculation shows that there is no solution  $(f, \lambda, \mu) \in \mathcal{S}$  corresponding to an eigenvalue satisfying  $\lambda^3 - \lambda^2 - 11\lambda - 7 = 0$ .

While, for  $\lambda = -1 \in \text{ev}(D)$  there is a solution in  $\mathcal{S}$ . Thus we have  $\Lambda_2(D) = \{-1\}$ . On the other hand, by routine calculation we obtain

$$P(\lambda) = 2(\lambda + 1)(2\lambda^2 + 6\lambda + 3)$$

and

$$\Lambda_1(D) = \{P(\lambda) = 0\} \setminus \text{ev}(D) = \{2\lambda^2 + 6\lambda + 3 = 0\} = \left\{ \frac{-3 \pm \sqrt{3}}{2} \right\}.$$

Consequently,

$$\text{QEC}(G) = \max \left\{ -1, \frac{-3 \pm \sqrt{3}}{2} \right\} = \frac{-3 + \sqrt{3}}{2}.$$

**Example 4.4.** Consider the complete graph  $K_n$  with  $n \geq 3$ . Then, for the distance matrix  $D$  we have

$$\det(\lambda - D) = (\lambda + 1)^{n-1}(\lambda - (n - 1))$$

and  $\Lambda_2(D) = \{-1\}$  by direct verification. On the other hand, we obtain

$$P(\lambda) = n(\lambda + 1)^{n-1}$$

and  $\Lambda_1(D) = \emptyset$ . Consequently,

$$\text{QEC}(K_n) = \max\{-1\} = -1.$$

#### 4.2. Use of spectra of distance matrices

For convenience we say that a finite graph  $G$  is of (CRS) if the distance matrix  $D = [d(x, y)]$  admits a constant row sum, i.e.,

$$\delta = \sum_{y \in V} d(x, y) \tag{21}$$

is a constant independent of  $x \in V$ . In order to avoid a trivial case, we consider a finite graph on two or more vertices.

**Lemma 4.5.** Let  $G = (V, E)$  be a finite graph with  $|V| \geq 2$ , and  $D$  the distance matrix. The following two conditions are equivalent:

- (i)  $G$  is of (CRS);
- (ii)  $\mathbf{1} \in C(V)$  is an eigenvector of  $D$ .

In that case,  $D\mathbf{1} = \delta\mathbf{1}$  with the constant  $\delta$  given by (21).

Following Brouwer–Cohen–Neumaier [4, Section 4.1], a connected graph  $G = (V, E)$  is called *distance degree regular* if for any  $k \geq 0$ , the number  $|\{y \in V; d(x, y) = k\}|$  is independent of  $x \in V$ . Apparently, a distance degree regular graph is of (CRS). Note that a distance-regular graph is distance degree regular, and that a distance degree regular graph is regular.

**Lemma 4.6.** *If the distance matrix  $D$  admits a constant row sum  $\delta$ , then  $\text{ev}(D) \subset [-\delta, \delta]$ . Moreover,  $\delta \in \text{ev}(D)$  and it is a simple eigenvalue.*

*Proof.* In general, every eigenvalue of a complex matrix  $A = [a_{ij}]$  lies in the centered disk with radius  $\max_i \sum_j |a_{ij}|$ . Then  $\text{ev}(D) \subset [-\delta, \delta]$  follows from the fact that every eigenvalue of the distance matrix  $D$  is real and the assumption that  $\delta$  in (21) is independent of  $x \in V$ . Moreover, from Lemma 4.5 we see that  $\delta \in \text{ev}(D)$ , that is,  $\delta$  is the largest eigenvalue of  $D$ . Since  $D$  is an irreducible matrix, it follows from the Perron-Frobenius theorem (see e.g., Bapat [3, Chapter 6], Horn–Johnson [10, Chapter 8]) that  $\delta$  is a simple eigenvalue.  $\square$

**Theorem 4.7.** *Let  $G = (V, E)$  be a graph of (CRS). Then  $\text{QEC}(G)$  coincides with the second largest eigenvalue of  $D$ . In particular, if the second largest eigenvalue of  $D$  is non-positive, the graph  $G$  is of QE class.*

*Proof.* By virtue of Lemma 4.6 we may arrange the eigenvalues of  $D$  as follows:

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-1} < \lambda_n = \delta.$$

Let  $\{f_k\}$  be an orthonormal basis of  $C(V)$  such that  $Df_k = \lambda_k f_k$  and  $f_n = \mathbf{1}/\|\mathbf{1}\|$ . Any  $f \in C(V)$  with  $\langle \mathbf{1}, f \rangle = 0$  admits an expression:

$$f = \sum_{k=1}^{n-1} \langle f_k, f \rangle f_k.$$

Then we have

$$\langle f, Df \rangle = \sum_{k=1}^{n-1} \lambda_k \langle f_k, f \rangle^2 \leq \lambda_{n-1} \sum_{k=1}^{n-1} \langle f_k, f \rangle^2 = \lambda_{n-1} \|f\|^2.$$

Since the equality holds for  $f = f_{n-1}$ , the maximum of  $\langle f, Df \rangle$  subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$  is  $\lambda_{n-1}$ . Consequently,  $\text{QEC}(G) = \lambda_{n-1}$ .  $\square$

It is noted that  $\lambda_{n-1} \leq \text{QEC}(G) \leq \lambda_n$  holds in general. For more on distance spectra, see e.g., an excellent survey by Aouchiche–Hansen [1].

**Example 4.8.** The complete graph  $K_n$  ( $n \geq 2$ ) is distance-regular. The eigenvalues of its distance matrix  $D$  are  $n-1$  with multiplicity 1 and  $-1$  with multiplicity  $n-1$ . It then follows from Theorem 4.7 that  $\text{QEC}(K_n) = -1$ .

**Example 4.9.** The cycle  $C_n$  ( $n \geq 3$ ) is distance-regular. The distance matrix  $D$  of  $C_n$  is a circular matrix and its eigenvalues are easily calculated, see e.g., Aouchiche–Hansen [1], Graovac–Jashari–Strunje [6]. In fact, for  $C_{2n+1}$  with  $n \geq 1$  the eigenvalues of  $D$  are

$$\lambda_0 = n(n+1), \quad \lambda_k = -\frac{1}{4 \cos^2 \frac{k\pi}{2n+1}}, \quad k = 1, 2, \dots, n,$$

where  $\lambda_0$  is multiplicity free and  $\lambda_k$  appears with multiplicity two for all  $k = 1, 2, \dots, n$ . Hence the second largest eigenvalues of  $D$  is found in  $\{\lambda_1, \dots, \lambda_n\}$  and we come to

$$\text{QEC}(C_{2n+1}) = -\frac{1}{4 \cos^2 \frac{\pi}{2n+1}}.$$

In particular,  $C_{2n+1}$  is of QE class. Similarly, for  $C_{2n}$  with  $n \geq 2$  the eigenvalues of  $D$  are

$$\lambda_0 = n^2, \quad \lambda_2 = \lambda_4 = \dots = \lambda_{2n-2} = 0, \quad \lambda_k = -\frac{1}{\sin^2 \frac{k\pi}{2n}}, \quad k = 1, 3, \dots, 2n-1.$$

Hence the second largest eigenvalues of  $D$  is 0 and  $\text{QEC}(C_{2n}) = 0$ . In particular,  $C_{2n}$  is of QE class too.

Now we give examples of graphs which are not of (CRS).

**Proposition 4.10.** For  $i = 1, 2$  let  $G_i = (V_i, E_i)$  be a finite graph with  $|V_i| \geq 2$ . Then  $G_1 \star G_2$  is not of (CRS).

*Proof.* Let  $m, n$  be integers such that  $|V_1| = m + 1$  and  $|V_2| = n + 1$ . Without loss of generality we may assume that  $m \leq n$ . We set

$$V_1 = \{o, x_1, x_2, \dots, x_m\}, \quad V_2 = \{o, y_1, y_2, \dots, y_n\},$$

where  $o$  is the common contact point of  $G_1 \star G_2$ . Then

$$V = \{o, x_1, \dots, x_m, y_1, \dots, y_n\}$$

becomes the set of vertices of  $G_1 \star G_2$ . Let  $D_1, D_2$  and  $D$  be the distance matrices of  $G_1, G_2$  and  $G_1 \star G_2$ , respectively. Now we compare two row sums of  $D$  given by

$$S_1 = \sum_{z \in V} (D)_{oz} = \sum_{i=1}^m (D)_{ox_i} + \sum_{j=1}^n (D)_{oy_j}, \tag{22}$$

$$S_2 = \sum_{z \in V} (D)_{x_1z} = (D)_{x_1o} + \sum_{i=1}^m (D)_{x_1x_i} + \sum_{j=1}^n (D)_{x_1y_j}. \tag{23}$$

Since  $x_i \in V_1$  and  $y_j \in V_2$  we have

$$S_1 = \sum_{i=1}^m d_1(o, x_i) + \sum_{j=1}^n d_2(o, y_j).$$

On the other hand, since  $(D)_{x_1y_j} = d_1(x_1, o) + d_2(o, y_j)$  we have

$$\begin{aligned} S_2 &= d_1(x_1, o) + \sum_{i=1}^m d_1(x_1, x_i) + \sum_{j=1}^n (d_1(x_1, o) + d_2(o, y_j)) \\ &= d_1(x_1, o) + \sum_{i=1}^m d_1(x_1, x_i) + nd_1(x_1, o) + \sum_{j=1}^n d_2(o, y_j). \end{aligned}$$



Then

$$S_2 - S_1 = nd_1(x_1, o) + \sum_{i=2}^m (d_1(x_1, x_i) - d_1(o, x_i)).$$

Since  $d_1(o, x_i) \leq d_1(o, x_1) + d_1(x_1, x_i)$  by the triangle inequality, we have

$$S_2 - S_1 \geq nd_1(x_1, o) - \sum_{i=2}^m d_1(o, x_1) = (n - m + 1)d_1(o, x_1) > 0.$$

Hence  $S_1 < S_2$ , which means that  $D$  does not admit a constant row sum. □

**Proposition 4.11.** *The complete bipartite graph  $K_{m,n}$  is of (CRS) if and only if  $m = n$ .*

**Proposition 4.12.** *The graphs of (CRS) on  $n$  vertices with  $1 \leq n \leq 5$  are  $K_n$  and  $C_n$ .*

The proofs of the above results are straightforward and omitted.


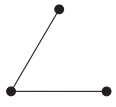
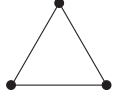
### 5. The graphs of QE class on $n$ vertices with $n \leq 5$

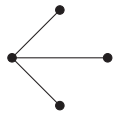
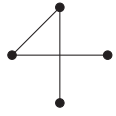
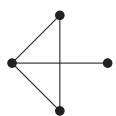
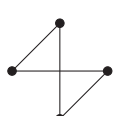
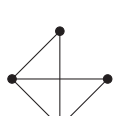
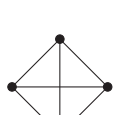
#### 5.1. Graphs on $n = 2, 3, 4$ vertices

**Theorem 5.1.** *Every graph on  $n$  vertices with  $n = 2, 3, 4$  is of QE class.*

*Proof.* For  $n = 2$  we have just one graph, which is  $K_2 \cong P_2$ . For  $n = 3$  we have  $P_3$  and  $K_3 \cong C_3$ . As is readily shown in Subsection 2.4, they are of QE class. For  $n = 4$ , the graphs No. 1–3 are the star products of smaller graphs of QE class, so they are also of QE class (Theorem 3.5). The graphs No. 4 ( $C_4$ ) and No. 6 ( $K_4$ ) are readily known to be of QE class. The graph No. 5 ( $K_4 \setminus \{e\}$ ) is of QE class by Theorem 3.9. □

The QE constants are shown in the following table, where we employ the list of finite connected graphs by McKay [16]. Calculation is routine and omitted, see also Subsection 5.3.

$n$	No.	graphs	edges	QE	comments	QE constants
2	1		1	QE	$K_2 \cong P_2$	-1
3	1		2	QE	$P_3$	$-\frac{2}{3}$
	2		3	QE	$K_3 \cong C_3$	-1

$n$	No.	graphs	edges	QE	comments	QE constants
4	1		3	QE	$K_{1,3}$	$-\frac{1}{2}$
	2		3	QE	$P_4$	$-\frac{2}{2 + \sqrt{2}}$
	3		4	QE	star	$-\frac{3}{3 + \sqrt{3}}$
	4		4	QE	$C_4 \cong K_2 \times K_2$	0
	5		5	QE	$K_4 \setminus \{e\}$	$-\frac{1}{2}$
	6		6	QE	$K_4$	-1

5.2. Graphs on  $n = 5$  vertices

There are 21 graphs. It is an easy task to list star products of smaller graphs of QE class. They are numbered by No. 1, 2, 3, 4, 5, 6, 7, 9, 11, 12, and 15. Next, we pick up graphs judged by means of general criteria. No. 8 ( $C_5$ ) and No. 21 ( $K_5$ ) are of QE class. No. 14 ( $K_5 \setminus K_3$ ) and No. 18 ( $K_5 \setminus P_3$ ) are of QE class by Theorems 3.12 and 3.11, respectively. No. 19 ( $K_5 \setminus \{e_1, e_2\}$ ) and No. 20 ( $K_5 \setminus \{e\}$ ) are of QE class by Theorems 3.9. We see from Theorem 2.8 that No. 10 ( $K_{2,3}$ ) is not of QE class. The rest are No. 13, 16, and 17, for which the QE constants are calculated directly from their distance matrices.

**No. 13** ( $K_5 \setminus P_5$ ) Under  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , we have

$$\langle f, Df \rangle = -\|f\|^2 + 2x_1x_4 + 2x_1x_5 + 2x_2x_5 + 2x_3x_4.$$

Then, using  $x_1 = -x_2 - x_3 - x_4 - x_5$ , we obtain

$$\begin{aligned} 2x_1x_4 + 2x_1x_5 + 2x_2x_5 + 2x_3x_4 &= -2(x_4 + x_5)^2 - 2x_2x_4 - 2x_3x_5 \\ &\leq -2(x_4 + x_5)^2 + (x_2^2 + x_4^2) + (x_3^2 + x_5^2) = -2(x_4 + x_5)^2 + 1 - x_1^2. \end{aligned}$$

Hence, under the conditions  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ , we have  $2x_1x_4 + 2x_1x_5 + 2x_2x_5 + 2x_3x_4 \leq 1$  and the equality holds for

$$x_1 = 0, \quad x_2 = x_5 = \pm \frac{1}{2}, \quad x_3 = x_4 = \mp \frac{1}{2}.$$

Consequently,  $\text{QEC}(K_5 \setminus P_4) = -1 + 1 = 0$ .

**No. 16** ( $K_5 \setminus P_4$ ) We need to find the maximum of

$$\langle f, Df \rangle = -\|f\|^2 + 2x_2x_4 + 2x_2x_5 + 2x_3x_5$$

subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ . Applying the method of Lagrange multipliers, we obtain

$$\max \{2x_2x_4 + 2x_2x_5 + 2x_3x_5; \|f\| = 1, \langle \mathbf{1}, f \rangle = 0\} = \frac{\sqrt{5} - 1}{2}.$$

Then,

$$\text{QEC}(K_5 \setminus P_4) = -1 + \frac{\sqrt{5} - 1}{2} = -\frac{2}{3 + \sqrt{5}}.$$

**No. 17** ( $K_5 \setminus \{P_3, e\}$ ) We need to find the maximum of

$$\langle f, Df \rangle = -\|f\|^2 + 2x_1x_4 + 2x_1x_5 + 2x_2x_3$$

subject to  $\|f\| = 1$  and  $\langle \mathbf{1}, f \rangle = 0$ . After a natural guess, setting

$$x_1 = \frac{2}{\sqrt{14}}, \quad x_2 = x_3 = -\frac{2}{\sqrt{14}}, \quad x_4 = x_5 = \frac{1}{\sqrt{14}},$$

we obtain

$$\langle f, Df \rangle = \frac{1}{7} > 0.$$

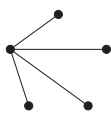
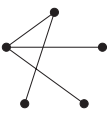
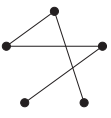


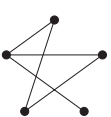
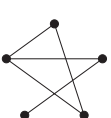
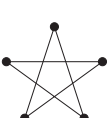
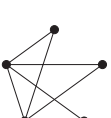

Therefore, this graph is not of QE class. The QE constant is calculated with the help of the method of Lagrange multipliers:

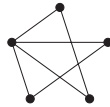
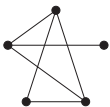
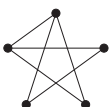







$$\text{QEC}(K_5 \setminus \{P_3, e\}) = \frac{4}{11 + \sqrt{161}}.$$

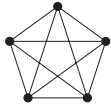
**Theorem 5.2.** *Among 21 graphs on 5 vertices there are two graphs which are not of QE class. They are No. 10 and 17.*

The above statement should be a folklore. In fact, the graph No. 10 is known as *Bożejko's obstruction*, see Hora–Obata [9, Chapter 2].

The following table summarizes the results. The QE constants are found by using the Schwartz inequality, the method of Lagrange multipliers and some elementary consideration, see also Subsection 5.3.

$n$	No.	graphs	edges	QE	comments	QE constants
5	1		4	QE	$K_{1,4}$	$-\frac{2}{5}$
	2		4	QE	star	$-2 + 2\lambda_1^*$ $\approx -0.4796$
	3		4	QE	$P_5$	$-\frac{4}{5 + \sqrt{5}}$
	4		5	QE	star	$-\frac{12}{15 + \sqrt{105}}$
	5		5	QE	star	$-\frac{2}{2 + \sqrt{2}}$
	6		5	QE	star	0
	7		5	QE	star	$-\frac{6}{6 + \sqrt{21}}$
	8		5	QE	$C_5$	$-\frac{2}{3 + \sqrt{5}}$
	9		6	QE	star	$-1 + \lambda_2^*$ $\approx -0.4463$
	10		6	NO	$K_{2,3}$	$\frac{2}{5}$

$n$	No.	graphs	edges	QE	comments	QE constants
5	11		6	QE	star	$-\frac{3}{5}$
	12		6	QE	star	$-\frac{4}{5 + \sqrt{5}}$
	13		6	QE	$K_5 \setminus P_5$	0
	14		7	QE	$K_5 \setminus K_3$	$-\frac{1}{5}$
	15		7	QE	star	$-\frac{4}{4 + \sqrt{6}}$
	16		7	QE	$K_5 \setminus P_4$	$-\frac{2}{3 + \sqrt{5}}$
	17		7	NO	$K_5 \setminus \{P_3, e\}$	$\frac{4}{11 + \sqrt{161}}$
	18		8	QE	$K_5 \setminus P_3$	$-\frac{5}{7 + 2\sqrt{6}}$
	19		8	QE	$K_5 \setminus \{e_1, e_2\}$	0
	20		9	QE	$K_5 \setminus \{e\}$	$-\frac{2}{5}$

$n$	No.	graphs	edges	QE	comments	QE constants
5	21		10	QE	$K_5$	-1

Note: (1)  $\lambda_1^*$  is the maximal real root of  $5\lambda^3 - 2\lambda^2 - 4\lambda + 2 = 0$ .

(2)  $\lambda_2^*$  is the maximal real root of  $5\lambda^3 + 3\lambda^2 - 5\lambda + 1 = 0$ .

### 5.3. Appendix

In practical calculation of the QE constant of a graph, we need to find the maximum of a certain quadratic function  $\varphi = \varphi(x_1, x_2, \dots, x_n)$ ,  $f = (x_1, x_2, \dots, x_n)$ , subject to

$$\begin{aligned} \langle f, f \rangle &= \|f\|^2 = x_1^2 + x_2^2 + \dots + x_n^2 = 1, \\ \langle \mathbf{1}, f \rangle &= x_1 + x_2 + \dots + x_n = 0. \end{aligned}$$

We record some results used in the previous arguments for convenience. For the proofs we only need to apply the Schwartz inequality and the method of Lagrange multipliers.

No.	$\varphi(x_1, \dots, x_n)$	parameters	cond max $\varphi$
1	$\left(\sum_{i=1}^r x_i\right)^2$	$1 \leq r \leq n$	$\frac{r(n-r)}{n}$
2	$\sum_{i=1}^r x_i^2$	$2 \leq r \leq n$	1
3	$\sum_{1 \leq i < j \leq r} 2x_i x_j$	$2 \leq r < n$	$\frac{(r-1)(n-r)}{n}$
4	$\sum_{i=1}^r 2x_{2i-1} x_{2i}$	$2 \leq r \leq \frac{n}{2}$	1
5	$2x_1 x_2 + 2x_1 x_3$	$n \geq 3$	$\frac{-2 + \sqrt{2(n-1)(n-2)}}{n}$
6	$2x_1^2 - 2x_2 x_3$	$n \geq 3$	$\frac{n + \sqrt{9n^2 - 24n}}{2n}$
7	$2x_1^2 + 2x_1 x_2 + 2x_2^2$	$n \geq 3$	$3 - \frac{6}{n}$

## Acknowledgements

NO is supported by JSPS KAKENHI 16H03939 and by JSPS Open Partnership Joint Research Project “Extremal graph theory, algebraic graph theory and mathematical approach to network science” (2017–18). AYZ is grateful for kind hospitality at the Graduate School of Information Sciences, Tohoku University and for the support by the Ministry of Research, Technology and Higher Education of the Republic of Indonesia through Sandwich-Like Program.

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