SHORT COMMUNICATION

Quadratic Embedding Constants of Wheel Graphs

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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, or equivalently if the quadratic embedding constant (QEC) of a graph is non-positive. The QEC of wheel graphs are calculated explicitly.

KEYWORDS: conditionally negative definite matrix, distance matrix, quadratic embedding, QE constant, wheel graph

1. Introduction

Let G = (V, E) be a (finite or infinite) connected graph and $D = [d(x, y)]_{x,y \in V}$ the distance matrix. An interesting question is whether or not D is conditional negative definite. Following [6] the QE constant of G is defined by

$$QEC(G) = \sup\{\langle f, Df \rangle \mid f \in C_0(V), \ \langle f, f \rangle = 1, \ \langle \mathbf{1}, f \rangle = 0\},\tag{1.1}$$

where $C_0(V)$ is the space of \mathbb{R} -valued functions on V with finite supports, **1** is the constant function taking value one on V, and $\langle \cdot, \cdot \rangle$ is the canonical inner product. By the Schoenberg theorem [7, 8] a graph G admits a quadratic embedding in a Hilbert space if and only if the distance matrix is conditionally negative definite, that is, $QEC(G) \leq 0$. Thus, the QE constant is an interesting characteristic of a graph from the point of view of Euclidean distance geometry [4]. In this paper we determine $QEC(W_n)$ for a wheel graph W_n on n + 1 vertices, $n \geq 3$. Other concrete examples of QEC(G) are found in [1–3, 5, 6]. The main result is stated in the following

Theorem 1.1. For $n \ge 3$ we have

$$QEC(W_n) = 0$$
 if *n* is even; $QEC(W_n) = -4\sin^2\frac{\pi}{2n}$ if *n* is odd. (1.2)

2. Join of Graphs

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two (finite or infinite, not necessarily connected) graphs that are disjoint, i.e., $V_1 \cap V_2 = \emptyset$. The *join* of G_1 and G_2 , denoted by $G_1 + G_2$, is a graph on $V = V_1 \cup V_2$ with edge set

$$E = E_1 \cup E_2 \cup \{\{x, y\} \mid x \in V_1, \ y \in V_2\}.$$

The graph join $G_1 + G_2$ is always connected, and is not locally finite unless both G_1 and G_2 are finite. Let A_1 and A_2 be the adjacency matrices of G_1 and G_2 , respectively. Then the adjacency matrix of $G = G_1 + G_2$ is given by

$$A = \begin{bmatrix} A_1 & J \\ J & A_2 \end{bmatrix},\tag{2.1}$$

where *J* is the matrix whose entries are all one (this symbol is used without explicitly mentioning its size). The diameter of $G = G_1 + G_2$ verifies $1 \le \text{diam}(G) \le 2$, and diam(G) = 1 occurs if and only if both G_1 and G_2 are complete graphs.

Proposition 2.1. Let G = (V, E) be a (finite or infinite) connected graph with diameter $1 \le \text{diam}(G) \le 2$. Let A be the adjacency matrix of G. Then,

$$\operatorname{QEC}(G) = -2 - \inf\{\langle f, Af \rangle \mid f \in C_0(V), \ \langle f, f \rangle = 1, \ \langle \mathbf{1}, f \rangle = 0\}.$$

$$(2.2)$$

Proof. Let *I* denote the identity matrix (this symbol is used without explicitly mentioning its size). For a graph with diameter $1 \le \text{diam}(G) \le 2$ we have the following obvious relation:

Received October 19, 2017; Accepted November 6, 2017

²⁰¹⁰ Mathematics Subject Classification: Primary 05C50, Secondary 05B20, 05C76.

This work is supported by JSPS Open Partnership Joint Research Project "Extremal Graph Theory, Algebraic Graph Theory and Mathematical Approach to Network Science" (2017–18) and JSPS Grant-in-Aid for Scientific Research (B) 16H03939.

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$$D = 2J - 2I - A. \tag{2.3}$$

Then, for any $f \in C_0(V)$ satisfying $\langle f, f \rangle = 1$ and $\langle \mathbf{1}, f \rangle = 0$, we obtain

$$\langle f, Df \rangle = \langle f, (2J - 2I - A)f \rangle = 2\langle f, Jf \rangle - 2\langle f, f \rangle - \langle f, Af \rangle = -2 - \langle f, Af \rangle,$$
(2.4)

where the obvious relation $\langle f, Jf \rangle = \langle \mathbf{1}, f \rangle^2$ is used. Taking the supremum of both sides of (2.4), we come to (2.2).

Proposition 2.2. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two arbitrary graphs that are disjoint, and A_1 and A_2 the adjacency matrices, respectively. Let $G = G_1 + G_2$ be their join, and let A and D be the adjacency and distance matrices of G, respectively. Then we have

$$D = 2J - 2I - A = \begin{bmatrix} 2J - 2I - A_1 & J \\ J & 2J - 2I - A_2 \end{bmatrix}$$
(2.5)

and

Since $\langle g, Jh \rangle$

$$QEC(G) = -2 - \inf\left\{ \langle g, A_1g \rangle + \langle h, A_2h \rangle - 2\langle \mathbf{1}, h \rangle^2 \middle| \begin{array}{l} g \in C_0(V_1), \ \langle g, g \rangle + \langle h, h \rangle = 1, \\ h \in C_0(V_2), \ \langle \mathbf{1}, g \rangle + \langle \mathbf{1}, h \rangle = 0 \end{array} \right\}.$$
(2.6)

Proof. (2.5) is a direct consequence of (2.1) and (2.3). Also from (2.1) we see that (2.2) becomes

$$\operatorname{QEC}(G) = -2 - \inf\left\{ \left\langle \begin{bmatrix} g \\ h \end{bmatrix}, \begin{bmatrix} A_1 & J \\ J & A_2 \end{bmatrix} \begin{bmatrix} g \\ h \end{bmatrix} \right\rangle \middle| \begin{array}{l} g \in C_0(V_1), \ \langle g, g \rangle + \langle h, h \rangle = 1, \\ h \in C_0(V_2), \ \langle \mathbf{1}, g \rangle + \langle \mathbf{1}, h \rangle = 0 \end{array} \right\}.$$

$$= \langle h, Jg \rangle = \langle \mathbf{1}, h \rangle \langle \mathbf{1}, g \rangle = -\langle \mathbf{1}, h \rangle^2 \text{ under condition } \langle \mathbf{1}, g \rangle + \langle \mathbf{1}, h \rangle = 0, \text{ we have}$$
$$\left\langle \begin{bmatrix} g \\ h \end{bmatrix}, \begin{bmatrix} A_1 & J \\ J & A_2 \end{bmatrix} \begin{bmatrix} g \\ h \end{bmatrix} \right\rangle = \langle g, A_1g \rangle + \langle h, A_2h \rangle - 2\langle \mathbf{1}, h \rangle^2,$$

from which (2.6) follows immediately.

3. Conditional Minimum

Let V be a finite set with $|V| = n \ge 3$, and T an arbitrary real symmetric matrix with index set V. We are interested in the conditional minimum:

$$M(T) = \min\{\langle f, Tf \rangle \mid f \in C(V), \ \langle f, f \rangle = 1, \ \langle \mathbf{1}, f \rangle = 0\},\tag{3.1}$$

where C(V) stands for the space of all \mathbb{R} -valued functions on V. Since V is a finite set with |V| = n, we have $C_0(V) = C(V) \cong \mathbb{R}^n$. Employing the method of Lagrange multipliers, we set

$$F(f,\lambda,\mu) = \langle f,Tf \rangle - \lambda(\langle f,f \rangle - 1) - \mu \langle \mathbf{1},f \rangle.$$
(3.2)

Let $\mathscr{S}(T)$ be the set of all stationary points of *F*, namely, the set of $(f, \lambda, \mu) \in C(V) \times \mathbb{R} \times \mathbb{R}$ at which all the partial derivatives of *F* vanish. After simple observation we see that $\mathscr{S}(T)$ consists of (f, λ, μ) satisfying

$$(T-\lambda)f = \frac{\mu}{2}\mathbf{1}, \quad \langle f, f \rangle = 1, \quad \langle \mathbf{1}, f \rangle = 0.$$
 (3.3)

The next result is useful for calculating QEC(G) for a finite graph G.

Lemma 3.1. $M(T) = \min \Lambda(T)$, where $\Lambda(T) = \{\lambda \in \mathbb{R} \mid (f, \lambda, \mu) \in \mathcal{S}(T) \text{ for some } f \in C(V) \text{ and } \mu \in \mathbb{R}\}.$

Proof. We first note that the conditions $\langle f, f \rangle = 1$ and $\langle \mathbf{1}, f \rangle = 0$ define a sphere of n - 2 dimension in $C(V) \cong \mathbb{R}^n$, which is a smooth compact manifold for $n \ge 3$. Since the quadratic function $\langle f, Tf \rangle$ is smooth, the conditional minimum M(T) is attained at a certain $f \in C(V)$ appearing in $\mathcal{S}(T)$. Namely,

$$M(T) = \min\{\langle f, Tf \rangle \mid f \in C(V) \text{ with } (f, \lambda, \mu) \in \mathscr{S}(T) \text{ for some } \lambda \in \mathbb{R} \text{ and } \mu \in \mathbb{R}\}.$$
(3.4)

On the other hand, for $(f, \lambda, \mu) \in \mathcal{S}(T)$ we have

$$\langle f, Tf \rangle = \left\langle f, \lambda f + \frac{\mu}{2} \mathbf{1} \right\rangle = \lambda \langle f, f \rangle + \frac{\mu}{2} \langle f, \mathbf{1} \rangle = \lambda.$$
(3.5)

Combining (3.4) and (3.5) we get the assertion.

Remark 3.2. In a similar manner as in the proof of Lemma 3.1 the following relation holds:

$$\max\{\langle f, Tf \rangle \mid f \in C(V), \ \langle f, f \rangle = 1, \ \langle \mathbf{1}, f \rangle = 0\} = \max \Lambda(T).$$

4. Wheel Graphs

Let $n \ge 3$. A wheel graph W_n is a graph on n + 1 vertices, defined as the join of a cycle C_n and a singleton graph K_1 . In what follows, the vertex set of W_n is taken to be $\{0, 1, 2, ..., n - 1, n\}$, where $\{0, 1, 2, ..., n - 1\}$ constitutes a cycle C_n with edge set $\{\{0, 1\}, \{1, 2\}, ..., \{n - 2, n - 1\}, \{n - 1, 0\}\}$ and the vertex n becomes a hub of the wheel. The adjacency matrices of C_n and K_1 are given respectively by

$$A_{1} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & 1 & \dots & 0 & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 1 & 0 \end{bmatrix}, \quad A_{2} = [0],$$

with which the adjacency matrix of W_n is of the form (2.1). Then, using Proposition 2.2 we obtain

$$\operatorname{QEC}(W_n) = -2 - \min\{\langle g, A_1g \rangle - 2h^2 \mid g \in \mathbb{R}^n, \ h \in \mathbb{R}, \ \langle g, g \rangle + h^2 = 1, \ \langle \mathbf{1}, g \rangle + h = 0\}.$$

$$(4.1)$$

We will calculate the conditional minimum in (4.1). Setting T to be the block diagonal matrix with blocks A_1 and -2I, we employ the method introduced in Sect. 3. Let δ be the set of all stationary points of

$$F(g,h,\lambda,\mu) = \langle g,A_1g \rangle - 2h^2 - \lambda(\langle g,g \rangle + h^2 - 1) - \mu(\langle \mathbf{1},g \rangle + h),$$
(4.2)

namely, the set of $(g, h, \lambda, \mu) \in \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}$ satisfying

$$(A_1 - \lambda)g = \frac{\mu}{2}\mathbf{1},$$
 (4.3)

$$(-2-\lambda)h = \frac{\mu}{2},\tag{4.4}$$

$$(g,g) + h^2 = 1,$$
 (4.5)

$$(1,g) + h = 0,$$
 (4.6)

and put $\Lambda = \{\lambda \in \mathbb{R} \mid (g, h, \lambda, \mu) \in \mathcal{S} \text{ for some } g \in \mathbb{R}^n, h \in \mathbb{R} \text{ and } \mu \in \mathbb{R}\}$. Then by Lemma 3.1 we have

$$\min\{\langle g, A_1g \rangle - 2h^2 \mid g \in \mathbb{R}^n, \ h \in \mathbb{R}, \ \langle g, g \rangle + h^2 = 1, \ \langle \mathbf{1}, g \rangle + h = 0\} = \min \Lambda.$$

$$(4.7)$$

Now we will determine the set Λ . Taking the inner product of (4.3) with **1**, we obtain $\langle \mathbf{1}, (A_1 - \lambda)g \rangle = (\mu/2) \langle \mathbf{1}, \mathbf{1} \rangle$. Then using $\langle \mathbf{1}, A_1g \rangle = \langle A_1\mathbf{1}, g \rangle = 2 \langle \mathbf{1}, g \rangle$, $\langle \mathbf{1}, \mathbf{1} \rangle = n$ and $\langle \mathbf{1}, g \rangle = -h$ by (4.6) we obtain

$$(\lambda - 2)h = \frac{\mu n}{2}.$$
(4.8)

On the other hand, for (4.3) we consider the difference equation:

$$g_{k-1} - \lambda g_k + g_{k+1} = \frac{\mu}{2}, \quad k \in \mathbb{Z}.$$
 (4.9)

Any solution to (4.9) satisfying the periodic condition $g_k = g_{n+k}$ gives rise to a solution $g = [g_0 \ g_1 \ \dots \ g_{n-1}]^T \in \mathbb{R}^n$ to (4.3), and vice versa. The characteristic equation of (4.9) is given by $\xi^2 - \lambda \xi + 1 = 0$, and we consider three cases according to the characteristic roots.

(Case 1) $\lambda = 2$ and the characteristic root is $\xi = 1$ (multiplicity two). We see first from (4.8) that $\mu = 0$. Using the characteristic root $\xi = 1$ and periodicity, we see that a general solution to (4.9) is given by $g_k = C$ (constant), and hence $g = C\mathbf{1}$. On the other hand, we have h = 0 by $\mu = 0$ and (4.4). Then (4.5) and (4.6) become $C^2\langle \mathbf{1}, \mathbf{1} \rangle = 1$ and $C\langle \mathbf{1}, \mathbf{1} \rangle = 0$, respectively, from which we come to contradiction. Consequently, $\lambda = 2 \notin \Lambda$.

(Case 2) $\lambda = -2$ and the characteristic root is $\xi = -1$ (multiplicity two). Note first that $\mu = 0$ by (4.4), and hence h = 0 by (4.8). In this case a general solution to (4.9) is given by $g_k = (C_1 + C_2k)(-1)^k$, where C_1 and C_2 are constants. Taking the periodicity into account, we obtain

$$g_k = \begin{cases} 0, & \text{if } n \text{ is odd,} \\ C_1(-1)^k, & \text{if } n \text{ is even.} \end{cases}$$

Then (4.5) is not fulfilled if *n* is odd, and it is fulfilled with $C_1 = 1/\sqrt{n}$ if *n* is even. Consequently, $\lambda = -2 \notin \Lambda$ if *n* is odd, and $\lambda = -2 \in \Lambda$ if *n* is even.

(Case 3) $\lambda \neq \pm 2$. Let α, β be the characteristic roots, where $\alpha \neq \beta, \alpha + \beta = \lambda$ and $\alpha\beta = 1$. Then a general solution

to (4.9) is given by

$$g_k = C_1 \alpha^k + C_2 \beta^k + \frac{\mu}{2(2-\lambda)},$$
(4.10)

where C_1 and C_2 are constants. The periodic conditions $g_0 = g_n$ and $g_1 = g_{n+1}$ give rise to

$$\begin{cases} (1 - \alpha^n)C_1 + (1 - \beta^n)C_2 = 0, \\ \alpha(1 - \alpha^n)C_1 + \beta(1 - \beta^n)C_2 = 0. \end{cases}$$
(4.11)

The determinant of the coefficient matrix is $(1 - \alpha^n)(1 - \beta^n)(\beta - \alpha)$.

(Case 3-1) $\alpha^n \neq 1$, also $\beta^n \neq 1$ by $\alpha\beta = 1$. We then see from (4.11) that $C_1 = C_2 = 0$. If $\mu = 0$, we have g = 0 by (4.10) and also h = 0 by (4.4). Then (4.5) is not fulfilled. Hence $\mu \neq 0$, and we have

$$g = \frac{\mu}{2(2-\lambda)}$$
1, $h = -\frac{\mu}{2(\lambda+2)}$

These satisfy (4.5) and (4.6) if and only if

$$\lambda = \frac{2-2n}{n+1} = -2 + \frac{4}{n+1}, \quad \mu^2 = \frac{64n}{(n+1)^3}.$$

Consequently, the above λ belongs to Λ . (This corresponds to the case of $g_k = \text{const.}$)

(Case 3-2) $\alpha^n = \beta^n = 1$. In this case we may set $\alpha = e^{2\pi i p/n}$ and $\beta = e^{-2\pi i p/n}$ with $p = 0, 1, 2, \dots, n-1$. Then,

$$\lambda = \alpha + \beta = 2\cos\frac{2p\pi}{n}.$$
(4.12)

Since $\lambda \neq \pm 2$ by assumption, we choose p from $\{1, 2, ..., n-1\} \setminus \{n/2\}$ and we have $\alpha, \beta \notin \{\pm 1\}$. Now we show that

$$\mu = 0, \quad h = 0, \quad g_k = \frac{\alpha^k + \beta^k}{\sqrt{2n}}$$

together with (4.12) satisfy (4.3)–(4.6). In fact, (4.3) follows since g_k in (4.10) is periodic for any choice of C_1 and C_2 . (4.4) is obvious. (4.5) follows from the obvious relations $1 + \alpha + \cdots + \alpha^{n-1} = 1 + \beta + \cdots + \beta^{n-1} = 0$. Similarly, (4.6) is verified. Consequently, every λ in (4.12) belongs to Λ .

Noting that $\lambda = -2$ is obtained by setting p = n/2 in (4.12), we may summarize the above three cases as follows:

$$\Lambda = \left\{-2 + \frac{4}{n+1}\right\} \cup \left\{2\cos\frac{2p\pi}{n} \mid 1 \le p \le n-1\right\}.$$

Now we compute $QEC(W_n) = -2 - \min \Lambda$, see (4.1) and (4.7). If *n* is even, we have $\min \Lambda = -2$ so that $QEC(W_n) = 0$. Suppose that *n* is odd, say, n = 2m - 1 with $m \ge 2$. Note that

$$\min\left\{2\cos\frac{2p\pi}{n} \mid 1 \le p \le n-1\right\} = 2\cos\frac{2m\pi}{2m-1} = -2\cos\frac{\pi}{2m-1} = -2 + 4\sin^2\frac{\pi}{2(2m-1)}.$$
 (4.13)

Using the obvious inequality $\sin \theta \le \theta$ for $\theta \ge 0$, we see by easy calculus that

$$4\sin^2\frac{\pi}{2(2m-1)} \le \frac{4}{(2m-1)+1}, \quad m \ge 2.$$

Therefore, min Λ is given by (4.13) and

QEC(
$$W_{2m-1}$$
) = $-2 - \min \Lambda = -4 \sin^2 \frac{\pi}{2(2m-1)} = -4 \sin^2 \frac{\pi}{2n}$,

which completes the proof of Theorem 1.1.

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