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ON EUCLIDEAN DISTANCE MATRICES OF GRAPHS*

GAŠPER JAKLIČ† AND JOLANDA MODIC‡

Abstract. In this paper, a relation between graph distance matrices and Euclidean distance matrices (EDM) is considered. It is proven that distance matrices of paths and cycles are EDMs. The proofs are constructive and the generating points of studied EDMs are given in a closed form. A generalization to weighted graphs (networks) is tackled.

Key words. Graph, Euclidean distance matrix, Distance, Eigenvalue.

AMS subject classifications. 15A18, 05C50, 05C12.

1. Introduction. A matrix $D \in \mathbb{R}^{n\times n}$ is a *Euclidean distance matrix (EDM)*, if there exist points $\boldsymbol{x}_i \in \mathbb{R}^r$, $i = 1, 2, \ldots, n$, such that $d_{ij} = \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$. The minimal possible r is called *an embedding dimension* (see, e.g., [3]). Euclidean distance matrices were introduced by Menger in 1928, later they were studied by Schoenberg [13], and other authors. They have many interesting properties, and are used in various applications in linear algebra, graph theory, and bioinformatics. A natural problem is to study configurations of points $\boldsymbol{x}_i$, where only distances between them are known.

Definition 1.1. A matrix $D = (d_{ij}) \in \mathbb{R}^{n\times n}$ is *hollow*, if $d_{ii} = 0$ for all $i = 1, 2, \ldots, n$.

There are various characterizations of EDMs.

Lemma 1.2. [8, Lemma 5.3] *Let a symmetric hollow matrix $D \in \mathbb{R}^{n\times n}$ have only one positive eigenvalue λ_1 and the corresponding eigenvector $\boldsymbol{e} := [1, 1, \ldots, 1]^T \in \mathbb{R}^n$. Then D is EDM.*

We will frequently use the following theorem.

Theorem 1.3. [8, Theorem 2.2] *Let $D \in \mathbb{R}^{n\times n}$ be a nonzero symmetric hollow matrix. Then D is EDM if and only if it has exactly one positive eigenvalue and there exists $\boldsymbol{w} \in \mathbb{R}^n$ such that $D\boldsymbol{w} = \boldsymbol{e}$ and $\boldsymbol{w}^T\boldsymbol{e} \geq 0$.*

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In order to obtain generating points $\boldsymbol{x}_i$ for an EDM matrix D, one can take a look at the singular value decomposition of Gower matrix

$$F = -\frac{1}{2}\left(I - \boldsymbol{e}\boldsymbol{s}^T\right) D \left(I - \boldsymbol{s}\boldsymbol{e}^T\right), \tag{1.1}$$

where $\boldsymbol{s}$ is a vector such that $\boldsymbol{s}^T\boldsymbol{e} = 1$ (see [1]). Since F is positive semidefinite, it can be written as $F = X^T X$ with $X = \operatorname{diag}(\sqrt{\sigma_i})\, U^T$, where $F = U\Sigma U^T$ is the singular value decomposition of F and $\Sigma = \operatorname{diag}(\sigma_i)$. The points $\boldsymbol{x}_i$ are obtained as columns of X.

An EDM matrix D is *circum-Euclidean* (CEDM) (also *spherical*) if there exists a realization of its generating points $\boldsymbol{x}_i$ that lie on the surface of some hypersphere [14]. Circum-Euclidean distance matrices are important because every EDM is a limit of CEDMs. This is analogous to the case of the cone of positive semidefinite matrices, where the interior of the cone consists of positive definite matrices.

CEDMs can be characterized by the following result.

THEOREM 1.4. [14, Theorem 3.4] *A Euclidean distance matrix $D \in \mathbb{R}^{n\times n}$ is CEDM if and only if there exist $\boldsymbol{s} \in \mathbb{R}^n$ and $\beta \in \mathbb{R}$, such that $D\boldsymbol{s} = \beta\boldsymbol{e}$ and $\boldsymbol{s}^T\boldsymbol{e} = 1$.*

If we choose $\boldsymbol{s} = 1/n\, \boldsymbol{e}$, the generating points of a CEDM lie on a hypersphere with center $\mathbf{0}$ and radius $R = \sqrt{\beta/2}$.

A nonzero EDM has only one positive eigenvalue λ_1, and the sum of its eigenvalues is zero. It is conjectured that any set of numbers that meet these conditions can be a spectrum of an EDM (see, e.g., [10, 11]).

In this paper we will study distance matrices, where the graph distance is used. Our goal is to cover basic graphs, paths and cycles, and give constructive proofs that their distance matrices are EDMs. This will enable study of more complex graphs and networks. A generalization to weighted graphs is considered. Here, instead of the graph distance, the minimal sum of edge weights over all possible paths between two vertices is used. Thus the problem considered becomes much harder.

Similar problems were studied in several papers. Line distance matrices were considered in [9, 12], cell matrices were introduced in [9], and distance matrices of weighted trees were studied in [2, 4].

The structure of the paper is as follows. In the next section, line distance matrices are presented and their relation to paths is analysed. In Section 3, we will apply the eigendecomposition of circulant matrices to study cycles and prove that their distance matrices are EDM. In Section 4, distance matrices of weighted cycles are considered. The paper is concluded by some remarks and ideas for future work.

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2. Paths. A graph distance matrix Dp_n for a path P_n is defined by $d_{ij} = |i - j|$, $i, j = 1, 2, \ldots, n$. Thus it is a symmetric Toeplitz matrix, generated by its first row $0, 1, 2, \ldots, n-1$.

A line distance matrix for parameters $t_1 < t_2 < \cdots < t_n$ is defined as $L = [\ell_{ij}]_{i,j}$ with $\ell_{ij} = |t_i - t_j|$ (see [12]). Hence Dp_n is a line distance matrix defined by the sequence $t_i = i$, $i = 1, 2, \ldots, n$. In [9] it was proven that line distance matrices are CEDMs.

Let L be a line distance matrix, associated with $t_1 < t_2 < \cdots < t_n$. The matrix $X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]$, $\boldsymbol{x}_i := [x_{i,1}, x_{i,2}, \ldots, x_{i,n}]^T$, where

$$x_{i,j} = \begin{cases} \frac{1}{2}\sqrt{t_{j+1} - t_j}, & j < i, \\ -\frac{1}{2}\sqrt{t_{j+1} - t_j}, & i \le j < n, \\ 0, & j = n, \end{cases} \tag{2.1}$$

is a realization matrix for L, i.e., its columns are generating points for EDM L. Its generating points $\boldsymbol{x}_i$ lie on the hypersphere with center $\mathbf{0}$ and radius $R = \frac{1}{2}\sqrt{t_n - t_1}$.

Since Dp_n is a line distance matrix, one can see that Dp_n is CEDM with generating points (2.1), lying on the hypersphere around the origin with radius $R = \frac{1}{2}\sqrt{n-1}$ and $t_i = i$.

Now let us consider weighted paths, i.e., paths P_n with edge weights $w_i > 0, i = 1, 2, \ldots, n-1$. Let $\boldsymbol{w} := [w_1, w_2, \ldots, w_{n-1}]$ and let $D^{\boldsymbol{w}}p_n$ denote the weighted path distance matrix. Here a path between every two vertices $v_i, v_j, i < j$, is unique, and its (generalized) distance is equal to the sum of weights $w_i + w_{i+1} + \cdots + w_{j-1}$. A weighted path distance matrix $D^{\boldsymbol{w}}p_n$ is a line distance matrix defined by the sequence $t_i := \sum_{k=1}^{i} w_{k-1}$, $i = 1, 2, \ldots, n$, where $w_0 := 0$. Thus the matrix $D^{\boldsymbol{w}}p_n$ is CEDM.

3. Cycles. A cycle is a graph C_n on n vertices consisting of a single closed directed walk. Let $V(G)$ denote the set of vertices of a graph G. Let us order vertices successively, and let us define the distance $d(u, v)$ between vertices $u, v \in V(C_n)$ as their graph distance, i.e., the length of the shortest path between them. Let us define the distance matrix $D_n := [d(u, v)]_{u,v \in V(C_n)}$. For example, for the cycle C_5 we obtain the distance matrix

$$D_5 = \begin{bmatrix} 0 & 1 & 2 & 2 & 1 \\ 1 & 0 & 1 & 2 & 2 \\ 2 & 1 & 0 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 \\ 1 & 2 & 2 & 1 & 0 \end{bmatrix}.$$

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Clearly, the matrix D_n is a circulant matrix (see [5]), generated by its first row $c_0, c_1, \ldots, c_{n-1}$, where we need to consider two possibilities for elements c_i:

$$0,\ 1,\ \ldots,\ \frac{n-1}{2},\ \frac{n-1}{2},\ \frac{n-1}{2}-1, \ldots, 1, \quad n \text{ odd},$$
$$0,\ 1,\ \ldots,\ \frac{n}{2}-1,\ \frac{n}{2},\ \frac{n}{2}-1, \ldots, 1, \quad n \text{ even}.$$

THEOREM 3.1. *The distance matrix D_n of a cycle is CEDM.*

Proof. Since D_n is a circulant matrix, it is well known (see, e.g., [5]) that it has eigenvalues

$$\lambda_{j+1} = \sum_{\ell=0}^{n-1} c_\ell \omega_j^\ell, \quad j = 0, 1, \ldots, n-1,$$

and the corresponding eigenvectors

$$\boldsymbol{v}_{j+1} := [1, w_j, w_j^2, \ldots, w_j^{n-1}]^T, \tag{3.1}$$

where $\omega_j := \exp(\mathrm{i}\, 2\pi j/n)$. Therefore,

$$\lambda_1 = \sum_{i=1}^{n-1} c_i = \frac{2n^2 - (1-(-1)^n)}{8}$$

and $\boldsymbol{v}_1 = \boldsymbol{e} = [1, 1, \ldots, 1]^T$. The symmetry in coefficients c_i and the facts that $\omega_j^{n-k} = \omega_j^k$ and

$$\omega_j^k + \omega_j^{-k} = 2\cos\left(\frac{2kj\pi}{n}\right)$$

yield

$$\begin{aligned}\lambda_{j+1} = &\sum_{k=1}^{\frac{n-1}{2}-\frac{1+(-1)^n}{4}} 2k\, \cos\left(\frac{2kj\pi}{n}\right) + (1+(-1)^n)\frac{n}{4}\cos j\pi = \\ &\frac{1}{2}\left(-1+(-1)^j \cos\frac{j\pi}{n}\right)\frac{1}{\sin^2\frac{j\pi}{n}} + (1+(-1)^n)\frac{n}{4}\cos j\pi.\end{aligned} \tag{3.2}$$

For n odd, we obtain

$$\lambda_{j+1} = \frac{1}{2}\left(-1+(-1)^j\cos\frac{j\pi}{n}\right)\frac{1}{\sin^2\frac{j\pi}{n}}.$$

Here the eigenvalues λ_j, $j = 2, 3, \ldots, n$ are obviously negative.

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For n even, the expression (3.2) simplifies to

$$\lambda_{j+1} = \frac{1}{2}\left(-1 - \frac{1}{\tan^2 \frac{j\pi}{n}} + \frac{\cos j\pi}{\sin^2 \frac{j\pi}{n}} + n\frac{\sin j\pi}{\tan \frac{j\pi}{n}}\right)$$
$$= \frac{1}{2}\left(-1 + (-1)^j\right)\frac{1}{\sin^2 \frac{j\pi}{n}}.$$

Thus $\lambda_j = 0$ for odd $j > 1$, and $\lambda_j < 0$ for j even.

Note that

$$\lambda_{j+1} = \lambda_{n-j+1}, \quad j = 1, 2, \ldots, n-1 \tag{3.3}$$

for arbitrary n.

Since D_n has only one positive eigenvalue with the corresponding eigenvector $\boldsymbol{e}$, by Lemma 1.2 it is EDM. By Theorem 1.4 with $\boldsymbol{s} = 1/n\,\boldsymbol{e}$ and $\beta = \lambda_1/n$, the matrix D_n is CEDM. ∎

An EDM with Perron eigenpair $(\lambda_1, \boldsymbol{e})$ is a *regular EDM*.

LEMMA 3.2. *A regular EDM with eigenpairs $(\lambda_i, \boldsymbol{u}_i)$, $i = 1, 2, \ldots, n$, has a realization matrix $X = (x_{i,j})_{i,j=1}^n$, where*

$$x_{i,j} := \begin{cases} 0, & i = 1, \\ \frac{\sqrt{-\lambda_i}}{\sqrt{2}\,\|\boldsymbol{u}_i\|}\, u_{j,i}, & i > 1. \end{cases} \tag{3.4}$$

The columns of X give generating points $\boldsymbol{x}_j$.

Proof. Let $D \in \mathbb{R}^{n\times n}$ be an EDM with Perron eigenpair $(\lambda_1, \boldsymbol{e})$ and let $(\lambda_i, \boldsymbol{u}_i)$, $i = 2, 3, \ldots, n$, be the rest of the eigenpairs. Its Gower matrix (1.1) for $\boldsymbol{s} = 1/n\,\boldsymbol{e}$ simplifies to

$$F = -\frac{1}{2}D + \frac{\lambda_1}{2n}\boldsymbol{e}\boldsymbol{e}^T. \tag{3.5}$$

Since $\boldsymbol{u}_1 = \boldsymbol{e}$ and $\boldsymbol{u}_j$, $j = 2, 3, \ldots, n$, are pairwise orthogonal,

$$F\boldsymbol{u}_j = -\frac{\lambda_j}{2}\boldsymbol{u}_j + \frac{\lambda_1}{2n}\left(\boldsymbol{e}^T\boldsymbol{u}_j\right)\boldsymbol{e} = \begin{cases} \boldsymbol{0}, & j = 1, \\ -\frac{\lambda_j}{2}\boldsymbol{u}_j, & j > 1. \end{cases}$$

Therefore, F has eigenpairs $(0, \boldsymbol{e})$ and $(-\frac{\lambda_j}{2}, \boldsymbol{u}_j)$, $j = 2, 3, \ldots, n$.

The matrix F is symmetric positive semidefinite, thus its singular value decomposition is equivalent to its eigenvalue decomposition

$$F = U\Lambda U^T,$$

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where

$$U = \left[\frac{\boldsymbol{e}}{\sqrt{n}}, \frac{\boldsymbol{u}_2}{\|\boldsymbol{u}_2\|}, \frac{\boldsymbol{u}_3}{\|\boldsymbol{u}_3\|}, \ldots, \frac{\boldsymbol{u}_n}{\|\boldsymbol{u}_n\|}\right], \quad \Lambda = \operatorname{diag}\left(0, -\frac{\lambda_2}{2}, -\frac{\lambda_3}{2}, \ldots, -\frac{\lambda_n}{2}\right).$$

From the decomposition $F = X^T X$ we obtain the realization matrix $X = \sqrt{\Lambda} U^T$, which completes the proof. ∎

Note that the Gower matrix of a cycle (3.5) is circulant since it is a sum of a circulant and a constant matrix. Now we can obtain generating points for the matrix D_n.

THEOREM 3.3. *The EDM D_n is generated by points $\boldsymbol{x}_i = [x_{1,i}, x_{2,i}, \ldots, x_{n,i}]^T \in \mathbb{R}^r$, $i = 1, 2, \ldots, n$, where*

$$x_{i,j} := \begin{cases} 0, & i = 1, \\ \sqrt{-\frac{\lambda_i}{n}} \cos\left(\frac{2\pi(i-1)(j-1)}{n}\right), & 1 < i < \frac{n+2}{2}, \\ \sqrt{-\frac{\lambda_i}{2n}} \cos\left(\frac{2\pi(i-1)(j-1)}{n}\right), & i = \frac{n+2}{2}, \\ \sqrt{-\frac{\lambda_i}{n}} \sin\left(\frac{2\pi(i-1)(j-1)}{n}\right), & i > \frac{n+2}{2}, \end{cases} \tag{3.6}$$

for $j = 1, 2, \ldots, n$, and its embedding dimension is

$$r = \begin{cases} n-1, & n \text{ odd}, \\ \frac{n}{2}, & n \text{ even}. \end{cases}$$

Proof. Let D_n be a circulant matrix with eigenvalues λ_{j+1} and the corresponding eigenvectors $\boldsymbol{v}_{j+1}$, $j = 0, 1, \ldots, n-1$, defined by (3.2) and (3.1). The eigenvectors $\boldsymbol{v}_j$, $j > 1$ are complex. But since the eigenvalues λ_j are double, we can replace the eigenvectors by suitable real eigenvectors $\boldsymbol{u}_j$,

$$\boldsymbol{u}_j = \begin{cases} \frac{1}{2}\left(\boldsymbol{v}_j + \boldsymbol{v}_{n-j+2}\right) = 2\left[\cos\left(\frac{2k\pi(j-1)}{n}\right)\right]^T_{k=0,1,\ldots,n-1}, & 2 \le j \le \frac{n+2}{2}, \\ \frac{1}{2\,\mathrm{i}}\left(\boldsymbol{v}_j - \boldsymbol{v}_{n-j+2}\right) = 2\left[\sin\left(\frac{2k\pi(j-1)}{n}\right)\right]^T_{k=0,1,\ldots,n-1}, & \frac{n+2}{2} < j \le n. \end{cases}$$

By Lemma 3.2 the realization matrix for D_n is of the form (3.4). It is easy to see that for n even, $\left\|\boldsymbol{u}_{\frac{n}{2}}\right\| = \sqrt{n}$, otherwise $\|\boldsymbol{u}_j\| = \sqrt{n/2}$. This completes the first part of the proof.

For n odd, the eigenvalues λ_j, $j = 2, 3, \ldots, n$, are negative. Since $x_{i,j} = 0$ for $i = 1$ and $j = 1, 2, \ldots, n$, the rank r of the realization matrix X is $r = n - 1$. When n is even, $\lambda_j = 0$ for odd $j > 0$ and $\lambda_j < 0$ for j even. Thus, in this case, $r = n/2$. ∎

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Let us have a detailed look at generating points (3.6). Since the matrix D_n is CEDM, its generating points lie on a hypersphere with center $\mathbf{0}$ and radius $R = \sqrt{\lambda_1/2n}$.

When n is odd, by (3.3) and $\sin(2k\pi) = \sin(2(1-k)\pi)$, $k \in \mathbb{Z}$, we get $\boldsymbol{x}_i = [0, \boldsymbol{y}_{i,1}, \boldsymbol{y}_{i,2}]^T$, where

$$\boldsymbol{y}_{i,1} = \begin{bmatrix} \sqrt{\frac{-\lambda_2}{n}} \cos\left(\frac{2\pi(i-1)\cdot 1}{n}\right) \\ \sqrt{\frac{-\lambda_3}{n}} \cos\left(\frac{2\pi(i-1)\cdot 2}{n}\right) \\ \vdots \\ \sqrt{\frac{-\lambda_{\frac{n-1}{2}}}{n}} \cos\left(\frac{2\pi(i-1)\cdot \frac{n-3}{2}}{n}\right) \\ \sqrt{\frac{-\lambda_{\frac{n+1}{2}}}{n}} \cos\left(\frac{2\pi(i-1)\cdot \frac{n-1}{2}}{n}\right) \end{bmatrix}, \quad \boldsymbol{y}_{i,2} = \begin{bmatrix} \sqrt{\frac{-\lambda_{\frac{n+1}{2}}}{n}} \sin\left(\frac{2\pi(i-1)\cdot \frac{n-1}{2}}{n}\right) \\ \sqrt{\frac{-\lambda_{\frac{n-1}{2}}}{n}} \sin\left(\frac{2\pi(i-1)\cdot \frac{n-3}{2}}{n}\right) \\ \vdots \\ \sqrt{\frac{-\lambda_3}{n}} \sin\left(\frac{2\pi(i-1)\cdot 2}{n}\right) \\ \sqrt{\frac{-\lambda_2}{n}} \sin\left(\frac{2\pi(i-1)\cdot 1}{n}\right) \end{bmatrix}.$$

This interpretation implies a nice symmetry.

For n even, $\lambda_j = 0$ for odd $j > 0$ and $\lambda_j < 0$ for j even. Thus, every other component of point $\boldsymbol{x}_i$ equals 0. The generating points can therefore be defined by $\boldsymbol{y}_i = [0, y_{2,i}, y_{4,i}, \ldots, y_{n,i}]^T \in \mathbb{R}^{n/2}$, where

$$y_{\ell,i} := \begin{cases} \sqrt{-\frac{\lambda_\ell}{n}} \cos\left(\frac{2\pi(i-1)(\ell-1)}{n}\right), & \ell = 2, 4, \ldots, \frac{n}{2}, \\ \sqrt{-\frac{\lambda_\ell}{n}} \sin\left(\frac{2\pi(i-1)(\ell-1)}{n}\right), & \ell = \frac{n}{2}+2, \frac{n}{2}+4, \ldots, n, \end{cases}$$

when $n/2$ is odd and

$$y_{\ell,i} := \begin{cases} \sqrt{-\frac{\lambda_\ell}{n}} \cos\left(\frac{2\pi(i-1)(\ell-1)}{n}\right), & \ell = 2, 4, \ldots, \frac{n}{2}-1, \\ (-1)^{i-1}\sqrt{-\frac{\lambda_\ell}{2n}}, & \ell = \frac{n}{2}+1, \\ \sqrt{-\frac{\lambda_\ell}{n}} \sin\left(\frac{2\pi(i-1)(\ell-1)}{n}\right), & \ell = \frac{n}{2}+3, \frac{n}{2}+5, \ldots, n, \end{cases}$$

for $n/2$ is even.

For $n = 3$ and $n = 4$, the generating points lie on a centered circle in a plane. Points for $n = 3$ form a regular triangle and for $n = 4$ they form a square with vertices lying on both axes. An example for $n = 6$ can be seen in Fig. 3.1. The embedding dimension in this case is $r = 3$ and the points lie on a sphere around origin with radius $R = \sqrt{3}/2$.

4. Weighted cycles. A generalization of distance matrices to weighted graphs, where the minimal sums of weights are used instead of graph distances, have been used in bioinformatics, for DNA sequence comparison, e.g., [12]. Clearly the analysis

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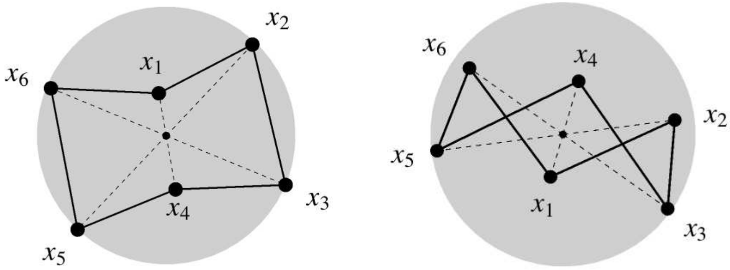

FIG. 3.1. *Spherical generating points of the cycle C_6 from two different angles.*

of such a matrix becomes a much harder problem, since it depends on the topology of a graph and on relations between edge weights. In Section 2, it was shown that a distance matrix of a weighted path is CEDM for every choice of positive weights. In this section, we will consider weighted cycles.

Let C_n be a cycle with edge weights $w_1, w_2, \ldots, w_n$ and let $\delta_{i,j} := \sum_{k=i}^{j-1} w_k$. Its distance matrix $D_n^{\boldsymbol{w}} := [d(i,j)]_{i,j}$ is defined by

$$d(i,j) := \min\{\delta_{i,j}, \delta_{1,n+1} - \delta_{i,j}\}, \quad i \leq j,$$

i.e., the shortest weighted distance on a cycle. For the distance between two vertices of the cycle only two possibilities need to be considered, for a general graph it is much more complicated.

First, let us consider the case where weights are natural numbers. By starting with a cycle, and using edge subdivisions (let $w_i = k \in \mathbb{N}$; add $k-1$ vertices to obtain a path with unit weights) we can transform the problem into the one, considered in Section 3.

THEOREM 4.1. *Let $D_n^{\boldsymbol{w}}$ be the distance matrix of a cycle C_n with weights $w_i \in \mathbb{N}$, $i = 1, 2, \ldots, n$. Then the matrix $D_n^{\boldsymbol{w}}$ is a CEDM.*

Now let us consider the general case where weights are positive reals. Here the problem is much harder. It turns out that we need to study several particular cases that depend on relations between weights. The number of cases increases exponentially with n. The following theorem covers the cases $n = 3, 4, 5$.

THEOREM 4.2. *Let $n \in \{3, 4, 5\}$. The distance matrix $D_n^{\boldsymbol{w}}$ of a cycle C_n with positive real weights is CEDM.*

Proof. Let us simplify the proof by using notation $a, b, c, \ldots$ instead of $w_1, w_2, \ldots$ (see Fig. 4.1). Further, let $D_n := D_n^{\boldsymbol{w}}$ denote a weighted distance matrix.

First, let us consider the case $n = 3$. From the definition of the distance matrix

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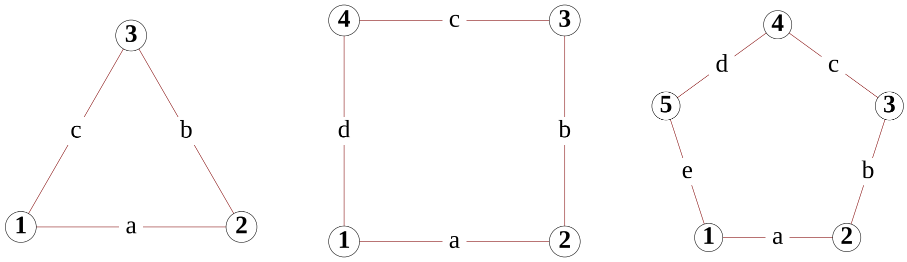

FIG. 4.1. *Cycles C_3, C_4 and C_5 with edge weights a, b, c, d, e.*

of the cycle C_3,

$$D_3 = \begin{bmatrix} 0 & \min\{a, b+c\} & \min\{c, a+b\} \\ \min\{a, b+c\} & 0 & \min\{b, a+c\} \\ \min\{c, a+b\} & \min\{b, a+c\} & 0 \end{bmatrix},$$

one can see that there are several possibilities based on different positions of weights and different relations between them. If we start with weights a and b, there are two options, $a \leq b$ an $a > b$. For each of these two options we have to study cases $b \leq c$ and $b > c$, etc. Further analysis is done as the decision tree in Fig. 4.2 implies.

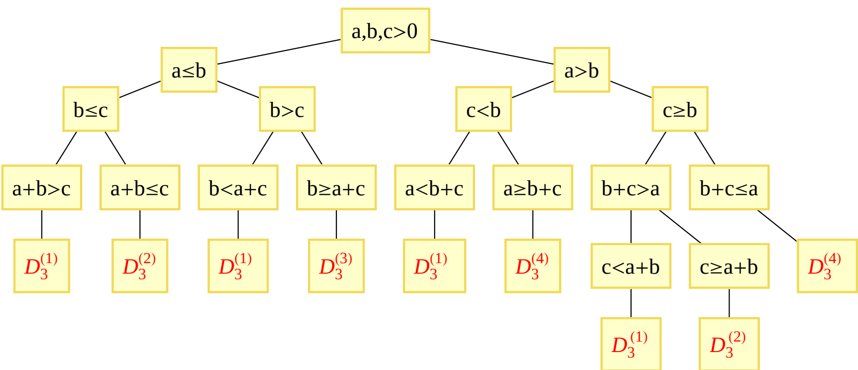

FIG. 4.2. *A decision tree for the case $n = 3$.*

We need to study four possible matrices,

$$D_3^{(1)} := \begin{bmatrix} 0 & a & c \\ a & 0 & b \\ c & b & 0 \end{bmatrix}, \quad a < b + c, \quad c < a + b, \quad b < a + c, \tag{4.1}$$

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and

$$D_3^{(2)} := \begin{bmatrix} 0 & a & a+b \\ a & 0 & b \\ a+b & b & 0 \end{bmatrix}, \quad a+b \le c,$$

$$D_3^{(3)} := \begin{bmatrix} 0 & a & c \\ a & 0 & a+c \\ c & a+c & 0 \end{bmatrix}, \quad a+c \le b,$$

$$D_3^{(4)} := \begin{bmatrix} 0 & b+c & c \\ b+c & 0 & b \\ c & b & 0 \end{bmatrix}, \quad b+c \le a.$$

But since a particular permutation of weights or vertices of the cycle yields the same distance matrix, there are only two matrices that need to be analysed, $D_3^{(1)}$ and one of matrices $D_3^{(2)}$, $D_3^{(3)}$ or $D_3^{(4)}$. Let us choose matrix $D_3^{(2)}$.

The matrix $D_3^{(2)}$ is a distance matrix of a weighted path on three vertices (see Fig. 4.3), and it is, as we have seen in Section 2, CEDM.

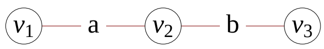

FIG. 4.3. *Weighted path corresponding to the matrix* $D_3^{(2)}$.

A simple computation yields the solution of the equation $D_3^{(1)}\boldsymbol{w} = \boldsymbol{e}$,

$$\boldsymbol{w} = \frac{1}{2abc}\left[b(a+c-b), c(a+b-c), a(b+c-a)\right]^T.$$

By (4.1) it follows $\boldsymbol{w}^T\boldsymbol{e} > 0$. The characteristic polynomial of the matrix $D_3^{(1)}$ is

$$p_{D_3^{(1)}}(\lambda) := -\lambda^3 + (a^2+b^2+c^2)\lambda + 2abc.$$

By applying Descartes' rule of signs on $p_{D_3^{(1)}}$, we can conclude that $D_3^{(1)}$ has exactly one positive eigenvalue. By Theorem 1.3, the matrix $D_3^{(1)}$ is EDM. Theorem 1.4 with $\beta = 1/(\boldsymbol{w}^T\boldsymbol{e})$ and $\boldsymbol{s} = 1/\beta\,\boldsymbol{w}$ implies that $D_3^{(1)}$ is CEDM.

An analogous analysis applies to the case $n = 4$. Here, there are eight different matrices that need to be studied. For a part of the analysis, see the decision tree in Fig. 4.4. Again, by using permutations, it turns out that only two cases need to be analysed,

$$D_4^{(1)} := \begin{bmatrix} 0 & a & a+b & a+b+c \\ a & 0 & b & b+c \\ a+b & b & 0 & c \\ a+b+c & b+c & c & 0 \end{bmatrix}, \quad \begin{array}{c} 0 < a \le b \le c \le d, \\ b+c \le a+d, \\ a+b+c \le d, \end{array}$$

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and

$$
D_4^{(2)} := \begin{bmatrix} 0 & a & a+b & d \\ a & 0 & b & b+c \\ a+b & b & 0 & c \\ d & b+c & c & 0 \end{bmatrix}, \qquad \begin{array}{c} 0 < a \le b \le c \le d, \\ b+c \le a+d, \\ d < a+b+c. \end{array} \tag{4.2}
$$

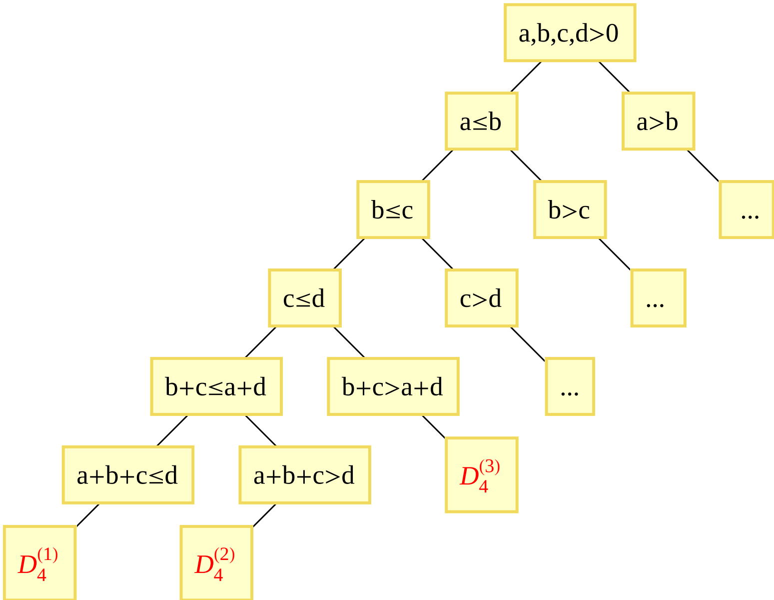

FIG. 4.4. *A decision tree for the case* $n = 4$.

The matrix $D_4^{(1)}$ is CEDM, since it is a distance matrix of a weighted path.

The solution of the equation $D_4^{(2)}\boldsymbol{w} = \boldsymbol{e}$ is

$$
\boldsymbol{w} = \frac{b}{\det(D_4^{(2)})} \begin{bmatrix} 2c(b+c-a-d) \\ (a+b-c-d)(a+b+c-d) \\ (a+b+c-d)(b+c-a-d) \\ 2a(a+b-c-d) \end{bmatrix},
$$

where

$$
\begin{aligned}
\det(D_4^{(2)}) = b\,(bc(b+c-a-d) + ab(a+b-c-d) + \\
+ b(b-d)(a+b+c-d) + 4ac(b-d))\,.
\end{aligned}
$$

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Clearly $\boldsymbol{w}^T\boldsymbol{e} \geq 0$ by the conditions on weights (4.2). If $\det(D_4^{(2)}) = 0$, the conditions (4.2) give $b = c = d = a$. Then

$$D_4^{(2)} = a \begin{bmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{bmatrix},$$

and $\boldsymbol{w}^T\boldsymbol{e} > 0$ holds true, since $\boldsymbol{w} = \frac{1}{2a}\left[1, 0, 1, 0\right]^T$ is a solution of the equation $D_4^{(2)}\boldsymbol{w} = \boldsymbol{e}$.

The characteristic polynomial of the matrix $D_4^{(2)}$ is

$$p_{D_4^{(2)}}(\lambda) := \lambda^4 + k_2\lambda^2 + k_1\lambda + \det(D_4^{(2)}),$$

where

$$k_2 := -(a^2 + b^2 + c^2 + d^2) - (a + b)^2 - (b + c)^2,$$
$$k_1 := -2((ab + cd)(a + b) + (ad + bc)(b + c)).$$

The Descartes' rule of signs implies that $D_4^{(2)}$ has exactly one positive eigenvalue. Thus $D_4^{(2)}$ is EDM by Theorem 1.3.

A simple analysis shows that $\boldsymbol{w}^T\boldsymbol{e} = 0$ could only hold for $b = c = d = a$. But since in this case $\det(D_4^{(2)}) = 0$, we conclude that $\boldsymbol{w}^T\boldsymbol{e} > 0$ always holds true. Theorem 1.4 with $\beta = 1/(\boldsymbol{w}^T\boldsymbol{e})$ and $\boldsymbol{s} = 1/\beta\,\boldsymbol{w}$ implies that $D_4^{(2)}$ is CEDM.

Now let us consider the last case, $n = 5$. Similarly as in the previous cases, it turns out that we need to study four particular matrices, together with relations on weights,

$$(4.3)\qquad D_5^{(1)} := \begin{bmatrix} 0 & a & a+b & d+e & e \\ a & 0 & b & b+c & a+e \\ a+b & b & 0 & c & c+d \\ d+e & b+c & c & 0 & d \\ e & a+e & c+d & d & 0 \end{bmatrix}, \quad \begin{array}{c} 0 < d \leq e \leq c \leq a \leq b, \\ a + b \leq c + d + e, \end{array}$$

$$D_5^{(2)} := \begin{bmatrix} 0 & a & c+d+e & d+e & e \\ a & 0 & b & b+c & a+e \\ c+d+e & b & 0 & c & c+d \\ d+e & b+c & c & 0 & d \\ e & a+e & c+d & d & 0 \end{bmatrix}, \quad \begin{array}{c} 0 < d \leq e \leq c \leq a \leq b, \\ c + d + e < a + b, \\ b \leq a + c + d + e, \\ b + c \leq a + d + e, \end{array}$$

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$$D_5^{(3)} := \begin{bmatrix} 0 & a & c+d+e & d+e & e \\ a & 0 & b & a+d+e & a+e \\ c+d+e & b & 0 & c & c+d \\ d+e & a+d+e & c & 0 & d \\ e & a+e & c+d & d & 0 \end{bmatrix},$$

with

$$\begin{aligned} &0 < d \leq e \leq c \leq a \leq b, && c+d+e < a+b, \\ &b \leq a+c+d+e, && a+d+e < b+c, \end{aligned}$$

and

$$D_5^{(4)} := \begin{bmatrix} 0 & a & c+d+e & d+e & e \\ a & 0 & a+c+d+e & a+d+e & a+e \\ c+d+e & a+c+d+e & 0 & c & c+d \\ d+e & a+d+e & c & 0 & d \\ e & a+e & c+d & d & 0 \end{bmatrix},$$

with

$$0 < d \leq e \leq c \leq a \leq b, \quad c+d+e < a+b, \quad a+c+d+e < b.$$

Clearly, the matrix $D_5^{(4)}$ is a distance matrix of a weighted path, thus it is CEDM.

The proofs for the matrices $D_5^{(2)}$ and $D_5^{(3)}$ are similar as in the previous cases, and will be omitted. It turns out that the proof for the matrix $D_5^{(1)}$ is not straightforward.

By solving the equation $D_5^{(1)}\boldsymbol{w} = \boldsymbol{e}$, and a very careful simplification of the results, it can be seen that $\boldsymbol{w}^T\boldsymbol{e} = \alpha/\det(D_5^{(1)})$, where

$$\begin{aligned} \alpha := \; & c(b+c+d-a-e)(a+b+e-c-d)(a+d+e-b-c)+ \\ & + d(c+d+e-a-b)(a+b+c-d-e)(a+b+e-c-d)+ \\ & + e(a+b+c-d-e)(b+c+d-a-e)(a+d+e-b-c)+ \\ & + a(c+d+e-a-b)(b+c+d-a-e)(a+b+e-c-d)+ \\ & + b(c+d+e-a-b)(a+b+c-d-e)(a+d+e-b-c), \end{aligned}$$

and

$$\begin{aligned} \det(D_5^{(1)}) = \frac{1}{2}\big(&(d+e)(b+c+d-e-a)(c+d+e-a-b)\cdot \\ &\cdot(d+e+a-b-c)(e+a+b-c-d)+ \\ &+b(a+b+c+d+e)(a+b+c-d-e)\cdot \\ &\cdot(c+d+e-a-b)(d+e+a-b-c)+ \\ &+(d+e-b)(a+b+c+d+e)(a+b+c-d-e)\cdot \\ &\cdot(b+c+d-e-a)(e+a+b-c-d)\big). \end{aligned} \tag{4.4}$$

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Together with limitations (4.3) and elegant forms of expressions this yields $\alpha \geq 0$ and $\det(D_5^{(1)}) \geq 0$. Thus $\boldsymbol{w}^T\boldsymbol{e} \geq 0$.

We are left with the possibility $\det(D_5^{(1)}) = 0$. Since all the summands in (4.4) are nonnegative, and are particular products of linear factors obtained from the matrix and limitations (4.3), a careful analysis of possibilities reveals that $\det(D_5^{(1)}) = 0$ if and only if $a = c$ and $b = d + e$. In this case, $\boldsymbol{w} = \frac{1}{a+d+e}\left[1, 0, 1, 0, 0\right]^T$ is the solution of the equation $D_5^{(1)}\boldsymbol{w} = \boldsymbol{e}$, and $\boldsymbol{w}^T\boldsymbol{e} > 0$ holds true.

The characteristic polynomial of the matrix $D_5^{(1)}$ is

$$p_{D_5^{(1)}}(\lambda) := -\lambda^5 + k_3\lambda^3 + k_2\lambda^2 + k_1\lambda + \det(D_5^{(1)}),$$

where

$$\begin{aligned}
k_3 &:= a(3a+2b) + b(3b+2c) + c(3c+2d) + d(3d+2e) + e(3e+2a),\\
k_2 &:= 2\left(ab(a+b+c+3d) + bc(b+c+d+3e) + cd(3a+c+d+e) + \right.\\
&\qquad \left. + ae(a+b+3c+e) + de(a+3b+d+e)\right),\\
k_1 &:= \frac{1}{2}\left(8(b+c)(a+b+c-d-e)(b+c+d-a-e)e + \right.\\
&\qquad +4e(c+d)(b+c+d-a-e)(a+d+e-b-c) + \\
&\qquad +(b+c+d-a-e)(a+b+e-c-d)\cdot\\
&\qquad\quad \cdot(a+b+c+e-d)(a+d+e-b-c) + \\
&\qquad +2(b+c)(b+c+d-a-e)\cdot\\
&\qquad\quad \cdot(a+b+e-c-d)(c+d+e-a-b) + \\
&\qquad +(a+b+c-d-e)(a+b+e-c-d)\cdot\\
&\qquad\quad \cdot(a+b+c+e-d)(c+d+e-a-b) + \\
&\qquad +2(b+c+d)(a+b+c-d-e)\cdot\\
&\qquad\quad \cdot(a+d+e-b-c)(c+d+e-a-b) + \\
&\qquad +4bc(a+b+c+d+e)(a+d+e-b-c) + \\
&\qquad \left. +2c(a+b+c+d+e)(a+b+e-c-d)(a+d+e-b-c)\right).
\end{aligned}$$

Descartes' rule of signs reveals that $D_5^{(1)}$ has exactly one positive eigenvalue, thus $D_5^{(1)}$ is EDM by Theorem 1.3. A lengthy computation shows that $\alpha = 0$ if and only if $\det(D_5^{(1)}) = 0$. Therefore, $\boldsymbol{w}^T\boldsymbol{e} > 0$ and by taking $\beta = 1/(\boldsymbol{w}^T\boldsymbol{e})$ and $\boldsymbol{s} = 1/\beta\,\boldsymbol{w}$, Theorem 1.4 implies that $D_5^{(1)}$ is CEDM. □

REMARK 4.3. The proof for the matrix $D_5^{(1)}$ is much harder than for the rest of the cases. Note that it is based on the elegant form of the determinant (4.4). In its basic form, this is a polynomial in 5 variables of the total degree 5. The main

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problem is how to prove that it is nonnegative on the domain, given by limitations (4.3). The idea on how to get such a nice form was obtained from the theory of polynomials, positive on compact semialgebraic sets (see, e.g., [6]). Although such a "Null/-Positivstellensatz" can not be used in our case, we expressed the polynomial as a linear combination (with unknown coefficients) of products of linear polynomials, obtained from the boundary of the domain. By a careful choice of linear factors, we got a solution with nonnegative coefficients. Therefrom the nonnegativity of the determinant is straightforward.

As can already be seen from the proof for the case $n = 5$, the analysis for larger n becomes more complex. But the proven results and numerical experiments suggest the following conjecture.

Conjecture 4.4. *The distance matrix $D_n^{\boldsymbol{w}}$ of a weighted cycle C_n is CEDM.*

5. Remarks. In [2], it was proven that distance matrices of trees are EDMs. The result holds true also for weighted trees. A proof can be found also in a recent monograph [4]. A similar result was proven for star-graphs and their generalization (see [9]). Based on presented results and numerical tests one may state a conjecture that the all-pairs shortest path matrix of a graph is EDM. But this is not true. For example, a distance matrix of the Möbius-Kantor graph (generalized Petersen graph GP(8,3), see Fig. 5.1) is not EDM, since its eigenvalues are

$$\left[-2\left(2+\sqrt{3}\right)\right]^4, [-2]^4, \left[-2\left(2-\sqrt{3}\right)\right]^4, [2]^3, 34.$$

The notation $[\cdot]^i$ indicates eigenvalue multiplicity.

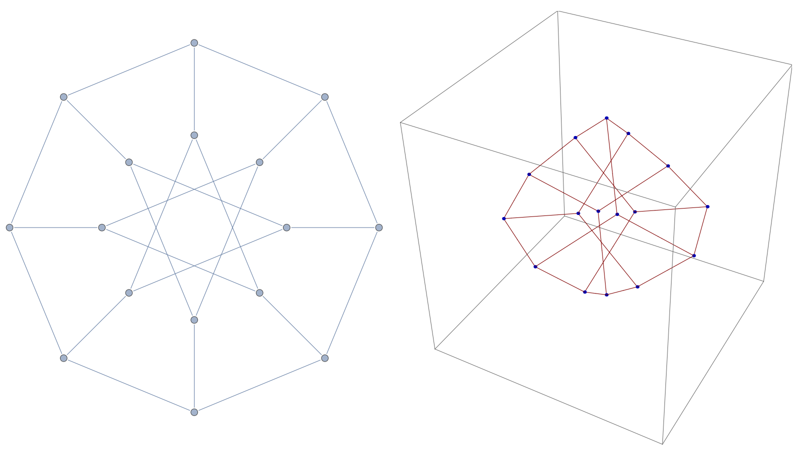

Fig. 5.1. *Möbius-Kantor graph and its 3D anisotropic embedding ([7]).*

Thus it is interesting to study particular families of graphs and their relations to

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EDMs. The analysis of graphs, derived from the path and cycle graph or star and k-star graph ([9]) would enable a more thorough study of the problem considered. A deeper insight into the relation between general graphs (and networks) and EDM structure could also be obtained by focusing on different products of graphs, e.g., Cartesian or Tensor product, and some broader graph classes, e.g., regular, bipartite or planar graphs.

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