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DISTANCE MATRIX AND ENERGY OF SEMIGRAPH

Surajit Kr. Nath, Ivan Gutman, and Ardhendu Kumar Nandi

Abstract. Let S be a semigraph. A definition of distance between the vertices of S is offered, for which the distance matrix of S is symmetric. The distance energy of S is defined as the sum of absolute values of the eigenvalues of the distance matrix. A few results on distance energy and distance-spectral radius of semigraphs of diameter 2 are established.

1. Introduction

Semigraphs are a kind of compromise between of the concept of hypergraphs [**2**] and graphs [**8**], or a kind of generalization of graphs. A semigraph S is defined [**15**] as an ordered pair $(\mathbf{V}, \mathbf{E})$, where $\mathbf{V} = \{v_1, v_2, \ldots, v_n\}$ is a non-empty (usually finite) set of elements called vertices of S, whereas $\mathbf{E} = \{e_1, e_2, \ldots, e_m\}$ is a set of ordered k-tuples of distinct vertices, called the edges of S. Each edge consists of a k-tuple of vertices, for various values of $k \geqslant 2$, satisfying the following conditions:

(a) Two edges have at most one vertex in common.

(b) Two edges $(x_1, x_2, \ldots, x_p)$ and $(y_1, y_2, \ldots, y_q)$ are considered to be sam if and only if $p = q$ and either $x_i = y_i$ for $1 \leqslant i \leqslant p$ or $x_i = y_{p+1-i}$ for $1 \leqslant i \leqslant p$.

Definition 1.1. Two vertices of a semigraph are adjacent if they belong to the same edge. The distance of such two vertices is equal to 1.

Definition 1.2. Two edges of a semigraph are incident if they they have a common vertex.

Definition 1.3. Let $e_1, e_2, \ldots, e_t$, $t \geqslant 2$, be distinct (mutually different) edges of a semigraph S, such that for $i = 1, 2, \ldots, t-1$, the edges e_i and e_{i+} are incident.

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Then these edges form a path in S, connecting the edges e_1 and e_t, whose length is t.

Definition 1.4. A semigraph is said to be connected if for any two of its edges there is a path connecting any them.

Definition 1.5. Let $e_1, e_2, \ldots, e_t,\ t \geqslant 2$, be a shortest path of the semigraph S, connecting the edges e_1 and e_t. Then the distance between the vertices belonging to e_1, but not to e_2, and the vertices belonging to e_t, but not to e_{t-1}, is t. If S is a connected semigraph, then the distance is well defined between any pair of its vertices.

The distance between the vertices u and v of the semigraph S will be denoted by $d_S(u, v)$.

At this point it should be noted that Definitions 1.1–1.5 are just one of the several possibilities that exist within the theory of semigraphs (for details see [**15**]). Based on the presently chosen distance between vertices (cf. Definitions 1.1 and 1.5), the distance matrix considered below will be symmetric, and its eigenvalues real–valued.

2. Matrix representations of semigraphs

The adjacency matrix of a semigraph S of order n is the square matrix $\mathbf{A}(S) = [a_{ij}]$ of order n whose elements are determined as follows [**5**]:

Definition 2.1. Let the vertex set of S be $\mathbf{X} = \{v_1, v_2, \ldots, v_n\}$. Let $e_i = (v_{i_1}, v_{i_2}, \ldots, v_{i_k})\,,\ i = 1, 2, \ldots, m$, be the edges of S, and recall that the value of k differs for different i. Then for $i = 1, 2, \ldots, m$, for $\ell = 1, 2, \ldots, k$, $a_{1,\ell} = \ell - 1$ and $a_{k,\ell} = k - \ell$. All other elements of $\mathbf{A}(S)$ are equal to zero.

Definition 2.1 was proposed by Deshpande et al. in 2017 [**5**] (see also an earlier work on this matter [**4**]). By means of it, the matrix $\mathbf{A}(S)$ is in a one-to-one correspondence with the semigraph S, i.e., reproduces all its structural details. Unfortunately, such a matrix is non-symmetric, having complex–valued eigenvalues. As a consequence, the energy of a semigraph cannot be defined in the usual manner, i.e., as the sum of absolute values of the eigenvalues of $\mathbf{A}(S)$ [**7, 12**]. Instead, in [**6**] the singular values of $\mathbf{A}(S)$ had to be employed. This creates a major shortcoming of the theory of semigraph energy, and significantly hinders its elaboration [**6**].

In order to avoid difficulties of this kind, we propose the following definition of the distance matrix $\mathbf{D}(S) = [d_{ij}]$ of a semigraph S.

Definition 2.2. Let S be a connected semigraph with vertex set $\mathbf{X} = \{v_1, v_2, \ldots, v_n\}$. Then the distance matrix of S is the square matrix $\mathbf{D}(S) = [d_{ij}]$ of order n, whose (i, j)-element is equal to $d_S(v_i, v_j)$, where the distance between vertices v_i and v_j is determined via Definitions 1.1–1.5. In addition, $d_{ii} = 0$ for all $i = 1, 2, \ldots, n$.

According to Definition 2.2, the distance matrix is symmetric, and therefore its eigenvalues are real–valued numbers.

EXAMPLE 2.1. Consider the 10-vertex semigraph S whose four edges are (v_1, v_2, v_3, v_4), (v_2, v_5, v_6), (v_3, v_6, v_7, v_8), (v_8, v_9, v_{10}). Then its distance matrix is:

$$\mathbf{D}(S) = \begin{bmatrix} 0 & 1 & 1 & 1 & 2 & 2 & 2 & 2 & 3 & 3 \\ 1 & 0 & 1 & 1 & 1 & 1 & 2 & 2 & 3 & 3 \\ 1 & 1 & 0 & 1 & 2 & 1 & 1 & 1 & 2 & 2 \\ 1 & 1 & 1 & 0 & 2 & 2 & 2 & 2 & 3 & 3 \\ 2 & 1 & 2 & 2 & 0 & 1 & 2 & 2 & 3 & 3 \\ 2 & 1 & 1 & 2 & 1 & 0 & 1 & 1 & 2 & 2 \\ 2 & 2 & 1 & 2 & 2 & 1 & 0 & 1 & 2 & 2 \\ 2 & 2 & 1 & 2 & 2 & 1 & 1 & 0 & 1 & 1 \\ 3 & 3 & 2 & 3 & 3 & 2 & 2 & 1 & 0 & 1 \\ 3 & 3 & 2 & 3 & 3 & 2 & 2 & 1 & 1 & 0 \end{bmatrix}$$

3. Distance spectrum and distance energy of semigraphs

The spectrum of the distance matrix of graphs has been extensively studied, see the survey [**1**] and the references cited therein. The distance energy of a graph, defined as the sum of absolute values of the eigenvalues of the distance matrix, was introduced in 2008 by Indulal et al. [**9**] and extensively studied since then, see the survey [**14**], the recent papers [**3, 10, 16, 17**], and the references cited therein.

Using the above defined distance matrix of a semigraph (Definition 2.2), the distance spectrum and distance energy of semigraphs can be conceived straightforwardly.

Let S be a connected semigraph, and $\mathbf{D}(S)$ its distance matrix. Denote by $\mu_1, \mu_2, \ldots, \mu_n$ its eigenvalues. These form the distance spectrum of S. Because $\mathbf{D}(S)$ is symmetric, the distance spectrum consists of real-valued numbers. Because the diagonal of $\mathbf{D}(S)$ is zero,

$$\sum_{i=1}^{n} \mu_i = 0\,.$$

In full analogy with the distance energy of a graph, the distance energy of a semigrah can now be defined as

$$E_D(S) = \sum_{i=1}^{n} |\mu_i|\,. \tag{3.1}$$

In what follows, we determine a few properties of $E_D(S)$ of semigraphs whose diameter is 2.

4. Distance energy of diameter 2 semigraphs

LEMMA 4.1. *Let S be a connected semigraph of order n and diameter 2. Let $e_1, e_2, \ldots, e_m$ be the edges of S, and $|e_i|$ the number of vertices in e_i. Then*

$$\sum_{i-1}^{n} \mu_i^2 = 4n^2 - 4n - 6\sum_{i=1}^{m} \binom{|e_i|}{2}\,. \tag{4.1}$$

PROOF. Since S has diameter 2, in its distance matrix there are $2\sum_{i=1}^{m}\binom{|e_i|}{2}$ elements equal to 1, n elements equal to 0, and $n^2-n-2\sum_{i=1}^{m}\binom{|e_i|}{2}$ elements equal to 2. Therefore,

$$\begin{aligned}\sum_{i-1}^{n}\mu_i^2 &= \sum_{i=1}^{n}(\mathbf{D}(S)^2)_{ii} = \sum_{i=1}^{n}\sum_{\ell=1}^{n} d(i,\ell)\,d(\ell,i) = \sum_{i=1}^{n}\sum_{\ell=1}^{n} d(i,\ell)^2 \\ &= 1^2\left[2\sum_{i=1}^{m}\binom{|e_i|}{2}\right] + 2^2\left[n^2-n-2\sum_{i=1}^{m}\binom{|e_i|}{2}\right],\end{aligned}$$

resulting in Eq. (4.1). □

Based on Lemma 4.1, applying a technique analogous to what McClelland used for estimating graph energy [**13**], we arrive at the following two theorems.

THEOREM 4.1. *Let S be a connected semigraph of order n and diameter 2. Using the notation from Lemma 4.1,*

$$ED(S) \geqslant \sqrt{4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2} + n(n-1)\,|\det\mathbf{D}(S)|^{2/n}} \tag{4.2}$$

with equality if and only if for all $1\leqslant i<j\leqslant n$, $|\mu_i\,\mu_j| = c$ for some fixed real number c.

PROOF. In view of Lemma 4.1,

$$\left(\sum_{i=1}|\mu_i|\right)^2 = \sum_{i=1}^{n}\mu_i^2 + \sum_{i\neq j}|\mu_i||\mu_j| = 4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2} + \sum_{i\neq j}|\mu_i\,\mu_j|\,.$$

The right–hand side summation in the above expression goes over $n(n-1)$ summands. Applying to it the geometric–arithmetic inequality, we get

$$\sum_{i\neq j}|\mu_i\,\mu_j| = n(n-1)\left[\frac{1}{n(n-1)}\sum_{i\neq j}|\mu_i\,\mu_j|\right] \geqslant n(n-1)\prod_{i\neq j}|\mu_i\,\mu_j|^{1/n(n-1)}$$

$$= \quad n(n-1)\prod_{i=1}^{n}|\mu_i|^{2/n} = n(n-1)\,\det|\mathbf{D}(S)|^{2/n}\,.$$

This yields

$$\left(\sum_{i=1}|\mu_i|\right)^2 \geqslant 4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2} + n(n-1)\,|\det\mathbf{D}(S)|^{2/p}$$

which by Eq. (3.1), directly implies the inequality (4.2). □

THEOREM 4.2. *Using the same notation is in Theorem 4.1,*

$$E_D(S) \leqslant \sqrt{4n^3 - 4n^2 - 6n \sum_{i=1}^{m} \binom{|e_i|}{2}} \tag{4.3}$$

with equality if and only if for all $1 \leqslant i \leqslant n$, $|\mu_i| = c$ *for some fixed real number* c.

PROOF. We start with the obvious relation

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \big(|\mu_i| - |\mu_j|\big)^2 \geqslant 0 \tag{4.4}$$

noting that equality holds if and only if all distance eigenvalues are mutually equal by absolute value. Expanding the left–hand side of (4.4), we get

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \big(|\mu_i| - |\mu_j|\big)^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \big(\mu_i^2 + \mu_j^2 - 2|\mu_i||\mu_j|\big)$$

$$= \quad n \sum_{i=1}^{n} \mu_i^2 + n \sum_{j=1}^{n} \mu_j^2 - 2 \left(\sum_{i=1} |\mu_i| \right) \left(\sum_{j=1} |\mu_j| \right)$$

which by Eqs. (3.1) and (4.1) yields

$$2n \left[4n^2 - 4n - 6 \sum_{i=1}^{m} \binom{|e_i|}{2} \right] - 2\, E_D(S)^2 \geqslant 0$$

from which (4.3) follows straightforwardly. □

LEMMA 4.2. *Let the distance eigenvalues of the semigraph* S *be labeled as* $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$. *If* S *is connected of diameter 2, then*

$$\mu_1 \geqslant \frac{2}{n} \left[n(n-1) - \sum_{i=1}^{m} \binom{|e_i|}{2} \right].$$

PROOF. According to the Rayleigh–Ritz variational principle, if Ω is any n-dimensional column vector, then

$$\frac{\Omega^T\, \mathbf{D}(S)\, \Omega}{\Omega^T\, \Omega} \leqslant \mu_1 \,.$$

Setting $\Omega = (1, 1, \ldots, 1)^T$, we get

$$\Omega^T\, \mathbf{D}(S)\, \Omega = \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} = 1 \cdot \left[2 \sum_{i=1}^{m} \binom{|e_i|}{2} \right] + 2 \cdot \left[n^2 - n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2} \right]$$

since the distance matrix has $2 \sum_{i=1}^{m} \binom{|e_i|}{2}$ elements equal to 1 and $n^2 - n - 2 \sum_{i=1}^{m} \binom{|e_i|}{2}$ elements equal to 2. In addition, $\Omega^T\, \Omega = n$.

Lemma 4.2 follows. □

Using Lemma 4.2, and following a proof technique invented by Koolen and Moulton [**11**] we obtain another upper bound for the distance energy of connected diameter 2 semigraphs.

THEOREM 4.3. *Using the same notation is in Theorems 4.1 and 4.2,*

$$E_D(S) \leqslant \frac{1}{n}\left[2n(n-1) - 2\sum_{i=1}^{m}\binom{|e_i|}{2} + \right.$$

$$\left.\sqrt{2n^2\,(n-1)\left[2n(n-1)-3\sum_{i=1}^{m}\binom{|e_i|}{2}\right]-4(n-1)\left[n(n-1)-\sum_{i=1}^{m}\binom{|e_i|}{2}\right]^2}\,\right].$$

PROOF. Applying the Cauchy–Schwarz inequality to the vectors $(1,1,\dots,1)$ and $(|\mu_2|,|\mu_3|,\dots,|\mu_n|)$, we obtain

$$\left(\sum_{i=2}^{n}|\mu_i|\right)^2 \leqslant (n-1)\sum_{i=2}^{n}\mu_i^2$$

from which, recalling that $\mu_1 > 0$,

$$\big(E_D(S)-\mu_1\big)^2 \leqslant (n-1)\left[\sum_{i=1}^{n}\mu_i^2-\mu_1^2\right] = (n-1)\left[4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2}-\mu_1^2\right]$$

i.e.,

$$E_D(S) \leqslant \mu_1 + \sqrt{(n-1)\left[4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2}-\mu_1^2\right]}. \tag{4.5}$$

Consider now the function

$$f(x) = x + \sqrt{(n-1)\left[4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2}-x^2\right]} \tag{4.6}$$

which is monotonically decreasing in the interval (a,b), where

$$a = \frac{2}{n}\left[n(n-1)-\sum_{i=1}^{m}\binom{|e_i|}{2}\right] \quad \text{and} \quad b = \sqrt{4n^2-4n-6\sum_{i=1}^{m}\binom{|e_i|}{2}}.$$

Therefore, inequality (4.5) remains valid if on the right-hand side (4.6) the variable x is replaced by the lover bound for μ_1 from Lemma 4.2 This results in Theorem 4.3. □

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Department of Mathematical Sciences, Bodoland University, Assam, India
E-mail address: `surajitnathe9@gmail.com`

Faculty of Science, University of Kragujevac, Kragujevac, Serbia
E-mail address: `gutman@kg.ac.rs`

Department of Mathematics, Basugoan College, Assam, India
E-mail address: `ardhendukumarnandi5@gmail.com`