Scientific paper

On Sum-Connectivity Matrix and Sum-Connectivity Energy of (Molecular) Graphs

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Received: 18-12-2009

This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

If G is a (molecular) graph with n vertices, and d_i is the degree of its i-th vertex, then the sum-connectivity matrix of G is the $n \times n$ matrix whose (i, j) -entry is equal to $1/\sqrt{d_i + d_j}$ if the i-th and the j-th vertices are adjacent and 0 otherwise. The sum-connectivity energy of a graph G is defined as the sum of the absolute values of the eigenvalues of the sum-connectivity matrix. Some properties including upper and lower bounds for the eigenvalues of the sum-connectivity matrix and the sum-connectivity energy are established, and the extremal cases are characterized.

Keywords: Randić connectivity index, Randić matrix, product-connectivity matrix, sum-connectivity matrix, sum-connectivity energy, sum-connectivity index

1. Introduction

Let G be a simple (molecular) graph with vertex set $V(G) = \{1, 2, ..., n\}$.[1,2] For a vertex $i \in V(G)$, d_i or $d_i(G)$ denotes the degree of i in G. Recall that $d_i = |\Gamma(i)|$, where $\Gamma(i)$ is the set of (first) neighbors of i in G. For vertices i and j of the graph G, $i \sim j$ means that i and j are adjacent, i.e., ij is an edge of G.

The product-connectivity matrix $\mathbf{R} = \mathbf{R}(G)$ of the graph G is defined as

$$\mathbf{R}_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}} & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

It was discussed by Rodríguez[3], Rodríguez and Sigarreta[4], Hogben[5] and Bozkurt *et al.*[6] under different names the weighted adjacency matrix[3], the degree-adjacency matrix[4], the normalized adjacency matrix[5] and the Randić matrix[6].

Recall that the product-connectivity index or the Randić index of the graph G is defined as in Ref. 7 and 8

$$R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}}.$$

The uses of the product-connectivity index and Randić-like indices in the structure-property-activity modeling is summarized by Todeschini and Consonni in their two Handbooks[9,10]. Similarly these authors also discussed in their Handbooks the role of graph-theoretical matrices in deriving molecular descriptors (topological indices) and in describing molecules from a topological point of view[11,12]. A useful summary of definitions and applications of graph-theoretical matrices in chemistry appeared recently[13].

In parallel to the definition of the product-connectivity index of Randić, the sum-connectivity index of the graph G is defined as in Ref. 14 and 15

$$S(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}}.$$

Sum-connectivity index belongs to a family of Randić-like indices. The uses of the sum-connectivity index in modeling a number of molecular properties is presented in the monograph entitled *Novel Molecular Structure Des-*

criptors – Theory and Applications I, edited by Gutman and Furtula[16].

Similarly to the product-connectivity matrix, the sum-connectivity matrix $\mathbf{S} = \mathbf{S}(G)$ of the (molecular) graph G is defined as

$$\mathbf{S}_{ij} = \begin{cases} \frac{1}{\sqrt{d_i + d_j}} & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

Obviously, $\mathbf{S}(G)$ is a symmetric real matrix. Thus its eigenvalues are all real. The sum-connectivity energy of a graph G is defined as the sum of the abosulute values of the eigenvalues of its sum-connectivity matrix of G.

The aim of this report is to study properties of the eigenvalues of the sum-connectivity matrix and the sum-connectivity energy, mainly upper and lower bounds of the largest and smallest eigenvalues, the spectral diameter (of the sum-connectivity matrix) and the sum-connectivity energy in terms of other structural invariants and complete characterizations for the extremal cases (for which the bounds are attained).

2. Definitions

The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of the graph G is defined as[12]

$$\mathbf{A}_{ij} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

For a square symmetric real matrix $\mathbf{B}$, its eigenvalues are all real. The energy of $\mathbf{B}$ is defined as the sum of absolute values of its eigenvalues, denoted by $E(\mathbf{B})$. The energy of the graph G is defined as[17] $E(G) = E(\mathbf{A}(G)) = \sum_{i=1}^{n}|\lambda i|$, where $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of $\mathbf{A}(G)$ arranged in a non-increasing manner. The product-connectivity energy or the Randić energy of the graph G is defined as[6] $RE(G) = E(\mathbf{R}(G))$. Similarly, the sum-connectivity energy of the graph G is defined as $SE(G) = E(\mathbf{S}(G)) = \sum_{i=1}^{n}|\mu_i|$, where $\mu_1, \mu_2, ..., \mu_n$ are the eigenvalues of $\mathbf{S}(G)$ arranged in a non-increasing manner.

Let $\mathrm{tr}(\mathbf{B})$ be the trace of the matrix $\mathbf{B}$. Then

$$\sum_{i=1}^{n} \mu_i = tr(\mathbf{S}) = \mathbf{0}, \tag{1}$$

$$\sum_{i=1}^{n} \mu_i^2 = tr(\mathbf{S}^2) = \sum_{i=1}^{n}\sum_{j=1}^{n}(\mathbf{S}_{ij})^2 = 2\sum_{i \sim j}\frac{1}{d_i + d_j}. \tag{2}$$

A graph is a semiregular graph of degrees r and s if it is a bipartite graph such that all vertices in one partite set have degree r and all vertices in the other partite set have degree s.

3. Properties of the Eigenvalues of the Sum-Connectivity Matrix

Obviously the spectrum of the sum-connectivity matrix of a disconnected graph is the union of the spectra of the sum-connectivity matrices of its components.

For a vector or matrix $\mathbf{X}$, $\mathbf{X}^T$ denotes its transpose.

Lemma 1.[18] Let $\mathbf{B}$ be a $k \times k$ non-negative irreducible symmetric matrix with exactly two distinct eigenvalues. Then $\mathbf{B} = \mathbf{u}\mathbf{u}^T + r\mathbf{I}_k$ for some positive column vector $\mathbf{u}$ and some r where $\mathbf{I}_k$ is the unit matrix of order k.

Proposition 1. Let G be a graph with $n \geq 2$ vertices. Then

$$\mu_1 \leq \sqrt{\frac{2(n-1)}{n}\sum_{i \sim j}\frac{1}{d_i + d_j}} \tag{3}$$

with equality if and only if G is an empty graph or a complete graph.

Proof. From (1) and applying the Cauchy-Schwarz inequality, we have

$$\mu_1^2 = \left(-\sum_{i=2}^{n}\mu_i\right)^2 \leq (n-1)\sum_{i=2}^{n}\mu_i^2.$$

From (2), we have

$$\mu_1^2 \leq (n-1)\left(2\sum_{i \sim j}\frac{1}{d_i + d_j} - \mu_1^2\right),$$

and then (3) follows.

It is obvious that (3) is an equality if G is an empty graph. Suppose that equality holds in (3) and G is nonempty. Then $\mu_2 = \cdots = \mu_n$ and thus from (1), $\mathbf{S}(G)$ has exactly two distinct eigenvalues, and by (1), the eigenvalues are not equal to zero. Let H be a component of G say $\mathbf{V}(H) = \{1, 2, ..., k\}$. Then $\mathbf{S}(H)$ has exactly two distinct eigenvalues. Note that $\mathbf{S}(H)$ is a non-negative irreducible symmetric matrix. By Lemma 1, $\mathbf{S}(H) = \mathbf{u}\mathbf{u}^T + r\mathbf{I}_k$ for some positive column vector $\mathbf{u}$ and some r. Since each diagonal entry of $\mathbf{S}(H)$ is zero, each entry of $\mathbf{u}$ is equal to $\sqrt{-r}$. Thus for $1 \leq i, j \leq k$ with $i \neq j$ all (i,j)-entries of $\mathbf{S}(H)$ are equal to $-r$, implying that G is a complete graph. Obviously, if G is a complete graph, then (3) is an equality.

We mention that

$$\sum_{i \sim j}\frac{1}{d_i + d_j}$$

is a particular case of the general sum-connectivity index[19].

Corollary 1. Let G be a graph with $n \geq 2$ vertices. Then

$$\mu_1 \le \sqrt{\frac{n-1}{n} R(G)}$$

with equality if and only if G is an empty graph or a complete graph.

Proof. It is easily seen that

$$\sum_{i\sim j} \frac{1}{d_i + d_j} \le \sum_{i\sim j} \frac{1}{2\sqrt{d_i d_j}} = \frac{R(G)}{2}$$

with equality if and only if every component of G is regular. Now the result follows from Proposition 1.

Corollary 2. Let G be a graph with $n \ge 2$ vertices. Then

$$\mu_1 \le \sqrt{\frac{n-1}{2}}$$

with equality if and only if G is a complete graph.

Proof. Note that[20] $R(G) \le \frac{n}{2}$. Then the result follows from Corollary 1.

Let G be a graph with n vertices. By Rayleigh's principle[21], an easy lower bound for μ_1 is given by

$$\mu_1 \ge \frac{2S(G)}{n}$$

with equality if and only if $\mathbf{S}(G)$ has equal row sums. For example, the sum-connectivity matrix of a regular graph or a semiregular graph has equal row sums.

Let G be a graph with $n \ge 2$ vertices. Then by Proposition 1 and the Perron-Frobenius theorem,

$$\mu_n \ge -\sqrt{\frac{2(n-1)}{n} \sum_{i\sim j} \frac{1}{d_i + d_j}}$$

with equality if and only if G is an empty graph or a 2-vertex complete graph.

A classic result is that the number of distinct eigenvalues of (the adjacency matrix of) a connected graph of diameter d is at least $d + 1$ [Theorem 3.13 in Ref. 22]. By the straightforward modification of the argument there to the sum-connectivity matrix, we have similar result as follows.

Lemma 2. Let G be a connected graph with diameter d. If $\mathbf{S}(G)$ has exactly k distinct eigenvalues, then $k \ge d + 1$.

Recall that $\mu_1 - \mu_n$ is the spectral diameter of $\mathbf{S} = \mathbf{S}(G)$. Consonni and Todeschini[23] investigated the use of the spectral diameter of molecular matrices.

Proposition 2. Let G be a graph with $n \ge 2$ vertices. Then

$$\mu_1 - \mu_n \le \mu_1 + \sqrt{2\sum_{i\sim j} \frac{1}{d_i + d_j} - \mu_1^2} \le 2\sqrt{\sum_{i\sim j} \frac{1}{d_i + d_j}} \quad (4)$$

with either equality if and only if G is an empty graph or G is a complete bipartite graph with possibly isolated vertices.

Proof. From (2) we have

$$\mu_1^2 + \mu_n^2 \le \sum_{i=1}^{n} \mu_i^2 = 2\sum_{i\sim j} \frac{1}{d_i + d_j}$$

and then

$$\mu_n \ge -\sqrt{2\sum_{i\sim j} \frac{1}{d_i + d_j} - \mu_1^2},$$

implying the first inequality, and the second inequality follows from the Cauchy-Schwarz inequality.

It is obvious that both inequalities in (4) are equalities if G is an empty graph. Suppose that either equality holds in (4) and G is non-empty. By discussion above and using (1), $\mathbf{S}(G)$ has exactly two nonzero eigenvalues μ_1 and $-\mu_1$ i.e., $\mathbf{S}(G)^2$ has exactly two distinct eigenvalues μ_1^2 (with multiplicity 2) and 0 (with multiplicity $n-2$). Thus there is (precisely) one component, say H with $k \ge 2$ vertices of G, for which $\mathbf{S}(H)^2$ has exactly two distinct eigenvalues μ_1^2 (with multiplicity 2) and 0 (with multiplicity $k-2$), and if $k < n$, then all other components are isolated vertices. Suppose first that H is not a bipartite graph. There is only one connected non-bipartite graph, i.e., the complete graph on three vertices, for which the eigenvalues of its sum-connectivity matrix are $1, -\frac{1}{2}, -\frac{1}{2}$, contradicting condition that $\mathbf{S}(G)$ has exactly two nonzero eigenvalues μ_1 and $-\mu_1$. Thus $k \ge 4$. By the Perron-Frobenius theorem, $\mathbf{S}(H)^2$ is irreducible. By Lemma 1, $\mathbf{S}(H)^2 = \mathbf{u}\mathbf{u}^T + r\mathbf{I}_k$ for some positive column vector $\mathbf{u}$ and some r. Thus there is an orthogonal matrix $\mathbf{U}$ such that $\mathbf{U}^T(\mathbf{u}\mathbf{u}^T + r\mathbf{I}_k)\mathbf{U} = \mathrm{diag}(\mu_1^2, 0, ..., 0, \mu_1^2)$. Let $\mathbf{y} = (y_1, ..., y_k)^T = \mathbf{U}^T\mathbf{u}$. Then $\mathbf{y}\mathbf{y}^T = \mathrm{diag}(\mu_1^2 - r, -r, ..., -r, \mu_1^2 - r)$. Note that the rank of $\mathbf{y}\mathbf{y}^T$ is at most one. Then $r = 0$, and thus $\mu_1^2 = 0$, a contradiction. Thus H must be a bipartite graph, and by Lemma 2, the diameter of H is at most two, implying that H is a complete bipartite graph. It follows that G is a complete bipartite graph with possibly isolated vertices. Conversely, if G is a complete bipartite graph with possibly isolated vertices, then $\mu_i = 0$ for $i = 2, ..., n-1$ and thus (4) is an equality.

Let G be a graph with $n \ge 2$ vertices. By the arguments as in Corollaries 1 and 2, we have

$$\mu_1 - \mu_n \le \sqrt{2R(G)}$$

$$\mu_1 - \mu_n \le \sqrt{n}$$

with the first equality if and only if G is an empty graph or G is a regular complete bipartite graph with possibly isolated vertices, and with the second equality if and only if G is a regular complete bipartite graph.

4. Properties of the Sum-Connectivity Energy

Proposition 3. Let G be a graph with n vertices. Then

$$SE(G) \le \sqrt{2n\sum_{i\sim j}\frac{1}{d_i+d_j}} \tag{5}$$

with equality if and only if G is an empty graph or a regular graph of degree one.

Proof. By Cauchy-Schwarz inequality and using (2), we have

$$SE(G)=\sum_{i=1}^{n}|\mu_i| = \sqrt{\left(\sum_{i=1}^{n}|\mu_i|\right)^2} \le \sqrt{n\sum_{i=1}^{n}\mu_i^2} = \sqrt{2n\sum_{i\sim j}\frac{1}{d_i+d_j}}.$$

Suppose that equality holds in (5). Then $\mu_1 = |\mu_2| = ... = |\mu_n|$. If $\mu_1 = 0$, then G is an empty graph. Suppose that $\mu_1 > 0$. From (1), we have $\mu_n < 0$ and then $\mathbf{S}(G)$ has exactly two distinct eigenvalues, implying that for any component H of G, $\mathbf{S}(H)$ has exactly two distinct eigenvalues μ_1 and $-\mu_1$. By the Perron-Frobenius theorem, the multiplicity of μ_1 as an eigenvalue of $\mathbf{S}(H)$ is one. Then $\mu_1 - (|V(H)| - 1)\,\mu_1 = 0$ i.e., $|V(H)| = 2$ and thus G is a regular graph of degree one. Conversely, if G is an empty graph or a regular graph of degree one, then it is easily seen that all eigenvalues of $\mathbf{S}(G)$ have equal abosolute values and thus (5) is an equality.

Let G be a graph with n vertices and m edges. Then by Proposition 3,

$$SE(G) \le \sqrt{nm}$$

with equality if and only if G is an empty graph or a regular graph of degree one.

Let G be a graph with n vertices. Then by Proposition 3 and the proof of Corollaries 1 and 2,

$$SE(G) \le \sqrt{nR(G)}$$

$$SE(G) \le \frac{n}{\sqrt{2}}$$

with the first equality if and only if G is an empty graph or a regular graph of degree one, and with the second equality if and only if G is a regular graph of degree one.

Proposition 4. Let G be a regular graph with n vertices and degree r. Then

$$\sqrt{2r}\,SE(G) = E(G).$$

Proof. Note that $\sqrt{2r}\,\mathbf{S}(G) = \mathbf{A}(G)$. Then $\sqrt{2r}\,\mu_i = \lambda_i$ for $i = 1, 2, ..., n$. Now the result follows by the definitions of $SE(G)$ and $E(G)$.

Proposition 5. Let G be a semiregular graph of degrees $r \ge 1$ and $s \ge 1$. Then

$$\sqrt{r+s}\,SE(G) = E(G).$$

Proof. Note that $\sqrt{r+s}\,\mathbf{S}(G) = \mathbf{A}(G)$. The result follows.

Proposition 6. Let G be a graph with n vertices. Then

$$SE(G) \ge 2\sqrt{\sum_{i\sim j}\frac{1}{d_i+d_j}} \tag{6}$$

with equality if and only if G is an empty graph or G is a complete bipartite graph with possibly isolated vertices.

Proof. From (1), we have $\sum_{i=1}^{n}\mu_i^2 + 2\sum_{1\le i<j\le n}\mu_i\mu_j = 0$,

i.e., $2\sum_{1\le i<j\le n}\mu_i\mu_j = -\sum_{i=1}^{n}\mu_i^2$. Thus

$$SE(G)^2 = \left(\sum_{i=1}^{n}|\mu_i|\right)^2 = \sum_{i=1}^{n}\mu_i^2 + 2\sum_{1\le i<j\le n}|\mu_i\mu_j| \ge \sum_{i=1}^{n}\mu_i^2 + 2\left|\sum_{1\le i<j\le n}\mu_i\mu_j\right| = 2\sum_{i=1}^{n}\mu_i^2,$$

which together with (2) implies that $SE(G)^2 \ge 4\sum_{i\sim j}\frac{1}{d_i+d_j}$. Then (6) follows.

It is obvious that (6) is an equality if G is an empty graph. Suppose that G is non-empty. From (1), we have $\mu_1 > 0$, $\mu_n < 0$. It is easily seen that equality holds in (6) if and only if there are not both positive and negative terms in the sum

$$\sum_{1\le i<j\le n}\mu_i\mu_j,$$

or equivalently, $\mu_i\,\mu_j \le 0$ for all i and j with $1 \le i < j \le n$, i.e., $\mu_i = 0$ for $i = 2, ..., n-1$. By the proof of Proposition 2, equality holds in (6) if and only if G is a complete bipartite graph with possibly isolated vertices.

Recall that the first Zagreb index of the graph G is defined[24–28] as $M_1(G) = \sum_{i=1}^{n} d_i^2$. Observe that[14] $M_1(G) = \sum_{i\sim j}(d_i + d_j)$.

Corollary 3. Let G be a graph with n vertices and $m \ge 1$ edges. Then

$$SE(G) \ge \frac{2m}{\sqrt{M_1(G)}}$$

with equality if and only if G is a complete bipartite graph with possibly isolated vertices.

Proof. By Cauchy-Schwarz inequality,

$$\sum_{i-j}\frac{1}{d_i+d_j}\cdot\sum_{i-j}(d_i+d_j)\geq\left(\sum_{i-j}\frac{1}{\sqrt{d_i+d_j}}\cdot\sqrt{d_i+d_j}\right)^2=m^2$$

with equality if and only if $d_i + d_j$ is a constant for all edges ij of G which is obviously satisfied by complete bipartite graphs with possibly isolated vertices. Then the result follows from Proposition 6.

Corollary 4. Let G be a triangle-free graph with n vertices and $m \geq 1$ edges. Then

$$SE(G)\geq 2\sqrt{\frac{m}{n}}$$

with equality if and only if G is a complete bipartite graph.

Proof. From Ref. 27 and 28, we have $M_1(G) \leq nm$ with equality if and only if G is a complete bipartite graph. The result follows from Corollary 3.

Let G be a tree with n vertices. By Corollary 4,

$$SE(G)\geq 2\sqrt{\frac{n-1}{n}}$$

with equality if and only if G is a star.

5. Concluding Remarks

In this report, we study some properties of the eigenvalues of the sum-connectivity matrix and sum-connectivity energy of (molecular) graphs. We give a number of upper and lower bounds for the largest eigenvalue, the spectral diameter and the sum-connectivity energy using some other structural invariants, such as the number of vertices (atoms) and their degrees (valencies) of a graph (molecule), and characterize the extremal cases. The bounds of a descriptor are important information of a molecule (graph) in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters.

6. Acknowledgements

This work was supported by the Guangdong Provincial Natural Science Foundation of China (Grant No. 8151063101000026) and by the Ministry of Science, Education and Sports of Croatia (Grant No. 098-1770495-2919).

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Povzetek

Če je G (molekulski) graf z n vozlišči in je d_i stopnja i-tega vozlišča, potem je matrika vsot povezljivosti grafa G $n \times n$ matrika, katere element (i,j) je enak $1/\sqrt{d_i + d_j}$, če sta vozlišči i in j sosednji in 0, če nista sosednji. Energija vsot-povezljivosti grafa G je definirana kot vsota absolutnih vrednosti lastnih vrednosti matrike vsot-povezljivosti. Vpeljane so nekatere lastnosti, vključno z zgornjo in spodnjo mejo lastnih vrednosti matrike vsot-povezljivosti in energije vsot-povezljivosti, in okarakterizirani ekstremni primeri.