Randić energy of digraphs

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**Abstract**

We assume that $D$ is a directed graph with vertex set $V(D) = \{v_1, \ldots, v_n\}$ and arc set $E(D)$. A VDB topological index $\varphi$ of $D$ is defined as

$$\varphi(D) = \frac{1}{2} \sum_{u \in V(D)} \varphi_{u_+, u_-},$$

where $d_{u_+}^+$ and $d_{u_-}^-$ denote the outdegree and indegree of vertices $u$ and $v$, respectively, and $\varphi_{i,j}$ is a bivariate symmetric function defined on nonnegative real numbers. Let $A_{\varphi} = A_{\varphi}(D)$ be the $n \times n$ general adjacency matrix defined as $[A_{\varphi}]_{ij} = \varphi_{i,j}\cdot$ if $e_{ij} \in E(D)$, and 0 otherwise. The energy of $D$ with respect to a VDB index $\varphi$ is defined as $E_{\varphi}(D) = \sum_{i=1}^{n} \sigma_i(A_{\varphi})$, where $\sigma_1(A_{\varphi}) \geq \sigma_2(A_{\varphi}) \geq \ldots \geq \sigma_n(A_{\varphi}) \geq 0$ are the singular values of the matrix $A_{\varphi}$.

We will show that in case $\varphi = R$ is the Randić index, the spectral norm of $A_{R}$ is equal to 1, and rank of $A_{R}$ is equal to rank of the adjacency matrix of $D$. Immediately after, we illustrate by means of examples, that these properties do not hold for most well-known VDB topological indices. Taking advantage of nice properties the Randić matrix has, we derive new upper and lower bounds for the Randić energy $E_{R}$ in digraphs. Some of these generalize known results for the Randić energy of graphs. Also, we deduce a new upper bound for the Randić energy of graphs in terms of rank, concretely, we show that $E_{R}(G) \leq \text{rank}(G)$ for all graphs $G$, and equality holds if and only if $G$ is a disjoint union of complete bipartite graphs.

1. Introduction

We assume that $D$ is a directed graph with vertex set $V = V(D)$ and $E = E(D)$, respectively. If $u, v \in V(D)$, we write $uv$ to specify an arc directed from $u$ to $v$. Given $u \in V(D)$, its indegree $d_{u_-}^+ = \{|u v \in E(D) : v \in V(D)\}$ (resp. outdegree $d_{u_+}^+ = \{|u v \in E(D) : v \in V(D)\}$). A vertex $u$ of $D$ is isolated if $d_{u_+}^+ = 0 = d_{u_+}^-$, a source vertex when $d_{u_+}^+ = 0 < d_{u_-}^+$ and a sink vertex when $d_{u_+}^+ = 0 < d_{u_-}^+$. An orientation of a graph $G$ is a directed graph $D$ that results from specifying a direction to all edges of $G$. An example of an orientation of a graph is the so called sink-source orientation, which is a digraph with vertex set consisting only of source and sink vertices.

A vertex-degree-based (VDB) topological index of a digraph $D$ was introduced in [21] as

$$\varphi(D) = \frac{1}{2} \sum_{u \in V(D)} \varphi_{u_+, u_-}, \quad (1)$$

where $\varphi_{i,j}$ is a bivariate symmetric function defined on nonnegative real numbers. We refer the reader to [21, 22] for recent results on VDB topological indices.

Assume that $V(D) = \{v_1, \ldots, v_n\}$ and let $A_{\varphi} = A_{\varphi}(D)$ be the $n \times n$ general adjacency matrix defined as

$$[A_{\varphi}]_{ij} = \begin{cases} \varphi_{i,j} d_{i_+}^+ d_{j_+}^- & \text{if } e_{ij} \in E(D) \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

In [23] the concept of energy of $D$ with respect to $\varphi$ was introduced as

$$E_{\varphi}(D) = \sum_{i=1}^{n} \sigma_i(A_{\varphi}) \quad (3)$$

where

$$\sigma_1(A_{\varphi}) \geq \sigma_2(A_{\varphi}) \geq \ldots \geq \sigma_n(A_{\varphi}) \geq 0$$

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are the singular values of the matrix $A_\phi$ (i.e. positive square roots of eigenvalues of $A_\phi A_\phi^T$). In case $\phi_{ij} \equiv 1$, $A_\phi$ coincides with the usual adjacency matrix $A$ of $D$, and $E_\phi(D)$ reduces to the energy $E(D) = \sum_{i=1}^{n} |\sigma_i|$. Recall that $E(D)$ was proposed by V. Nikiforov [24] as a natural generalization of the energy of a graph $G$, defined in terms of eigenvalues of its adjacency matrix as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ [10, 17]. Note that in this case, the eigenvalues of $AA^T = A^2$ are $\lambda_1^2, \ldots, \lambda_n^2$, and so the singular values of $A$ are precisely $|\lambda_1|, \ldots, |\lambda_n|$.

It is relevant to mention that definition (3) generalizes graph energy associated to $\phi$, as proposed in [9], and eventually investigated in several recent papers [12, 13, 18, 27]. Perhaps the most important VDB topological index and certainly the most widely applied in chemistry is the Randić index [15, 16, 25, 26], which we will denote by $R$. The energy associated to the Randić index is called Randić energy, introduced in [3, 4] for graphs, and currently under study [2, 8, 11]. However, for general digraphs, research on $E_\phi$ just started in [23]. Naturally, innumerable problems arise in the study of $E_\phi$ over the large class of digraphs, which strictly contains the class of graphs (identified as symmetric digraphs).

Given the significance of the Randić index, we dedicate our attention to the paper to the energy of digraphs. It comes out that the Randić matrix $A_R$ of a digraph $D$ has remarkable properties, namely, the spectral norm of $A_R$ is equal to 1, and rank of $A_R$ is equal to rank of $A$ (see Lemmas 2.3 and 2.4). Immediately after, we illustrate by means of examples (Example 2.5 and Example 2.6), that these properties do not hold for most well-known VDB topological indices. As a consequence, we derive new upper and lower bounds for the Randić energy $E_R$ in digraphs. Some of these generalize known results for the Randić energy of graphs [3, 6, 19]. Also, we deduce a new upper bound for the Randić energy of graphs in terms of rank, concretely, we prove that $E_R(G) \leq \text{rank}(G)$ for all graphs $G$, and equality holds if and only if $G$ is a disjoint union of complete bipartite graphs.

2. Randić matrix of a digraph

If we replace $\phi_{ij}$ by $\frac{1}{\sqrt{d_i d_j}}$ in (1) we obtain the Randić index of a digraph $D$:

$$R(D) = R(D) = \frac{1}{2} \sum_{v \in V(D)} \frac{1}{\sqrt{d_i d_j}}$$

In this case, the general adjacency matrix $A_R$ of $D$ is called Randić matrix of $D$, and it is defined as

$$[A_R]_{ij} = \left\{ \begin{array}{ll} \frac{1}{\sqrt{d_i d_j}} & \text{if } e_{ij} \in E(D) \\ 0 & \text{otherwise.} \end{array} \right.$$

In order to study the Randić matrix $A_R$, let us recall the concept of splitting digraph [23]. Let $D$ be a digraph and consider the set

$$T = \{ u \in V(D) : \exists d_j \neq 0 \}$$

of tails of $D$ and the set

$$H = \{ u \in V(D) : \exists d_j = 0 \}$$

of heads of $D$. The splitting digraph $S_D$ of $D$ is the digraph with vertex set

$$V(S_D) = \{ u^H : u \in T \} \cup \{ u^H : u \in H \}.$$

The arc set of $S_D$ is given by $E(S_D) = \{ u^H v^H : uv \in E \}$. We denote by $H_D$ the underlying graph of $S_D$.

Example 2.1. Let $Q$ be the digraph illustrated in Fig. 1. The set of tails of $Q$ is $T = \{ u_1, u_2 \}$, and the set of heads of $Q$ is $H = \{ u_3, u_4 \}$. Then the vertex set of $S_Q$ is

![Fig. 1. Digraph $Q$, its splitting digraph $S_Q$ and its underlying graph $H_Q$ in Example 2.1.](image)

$$V(S_Q) = \{ u_1^H, u_2^H, u_3^H, u_4^H \}$$

and

$$E(S_Q) = \{ u_1^H u_2^H, u_1^H u_3^H, u_1^H u_4^H, u_2^H u_3^H \}.$$

The arc set of $S_Q$ and its underlying graph $H_Q$ is shown in Fig. 2. Note that every vertex of the splitting digraph $S_D$ of a digraph $D$ is a source vertex or a sink vertex.

Now we can show one first important spectral property $A_R$ has.

Lemma 2.3. Let $D$ be a digraph (with at least one arc) and Randić matrix $A_R$. Then $\sigma_1(A_R) = 1$.

Proof. By [20, Theorem 2.1], the spectral radius of the matrix $A_R(H_D)$ is $\rho(A_R(H_D)) = 1$. It follows from [23, Lemma 3.2] that $\sigma_1(A_R) = \rho(A_R(H_D)) = 1$. □

On the other hand, recall that the rank of a digraph $D$ is the rank of the adjacency matrix $A$ of $D$. Namely, $\text{rank}(D) = \text{rank}(A)$. Another interesting property the Randić matrix has is that its rank coincides with the rank of the adjacency matrix of the digraph.

Lemma 2.4. Let $D$ be a digraph. Then $\text{rank}(A_R) = \text{rank}(D)$.

Proof. Given a $n$-vertex digraph $D$, let $D^+$ (resp. $D^-$) be the $n \times n$ diagonal matrix whose $j$-th diagonal entry is $\max \{ 1, d_j^+ \}$ (resp. $\max \{ 1, d_j^- \}$). By direct matrix multiplication we can see that $A_R = (D^+)^{-1/2} A (D^-)^{-1/2}$. Since the matrices $D^+$ and $D^-$ are nonsingular, and multiplying by a nonsingular matrix does not change the rank of $A$, it follows $\text{rank}(A_R) = \text{rank}(A) = \text{rank}(D)$. □

We are interested in those VDB topological indices $\phi$ such that $\sigma_1(A_\phi) = 1$ and $\text{rank}(A_\phi) = \text{rank}(A)$, for all digraphs $D$. Certainly, the Randić index $R$ is one of them. The general Randić index $R_n$ is obtained...
from the function \( \varphi_{ij} = (i) a^r \), where \( a \in \mathbb{R} \). In particular, \( R = R_{-\frac{1}{2}} \). A similar proof to the proof of Lemma 2.4 shows that \( \text{rank}(A_{R_a}) = \text{rank}(A) \), for all \( a \in \mathbb{R} \). However, the only value for which \( \sigma_1(A_{R_a}) = 1 \) is \( a = -\frac{1}{2} \), as we shall see in our next example.

Recall that a digraph \( D \) is \( r \)-regular if \( d^+_v = d^-_v = r \) for each vertex \( v \). If \( D \) is \( r \)-regular, then \( \sigma_1(A) = r \) (see [5]).

Example 2.5. Let \( \varphi \) be a VDB topological index and let \( D \) be a \( r \)-regular digraph with adjacency matrix \( A \) and general adjacency matrix \( A_{\varphi} \). By (2) it follows that \( A_{\varphi} = \varphi, A \). Consequently, \( \sigma_1(A_{\varphi}) = \varphi, A = \varphi, \sigma_1(A) = r \). It is easy to check that for most well-known VDB topological indices different from the Randić index, \( r \varphi, \varphi \neq 1 \). For instance, in the general Randić index, \( \varphi_{ij} = (i) a^r \). Hence \( r \varphi, \varphi = r^{2a+1} \neq 1 \), except for \( a = -\frac{1}{2} \). Another example is the general sum-connectivity index obtained from the function \( \varphi_{ij} = (i + j)^a \). In this case \( r \varphi, \varphi = 2^{a+1} \neq 1 \), except for \( a = -\frac{1}{2} \).

The Randić index, induced by the function \( \varphi_{ij} = \frac{1}{\sqrt{1 + d^-_i d^-_j}} \), is an exception since \( r \varphi, \varphi = 1 \). However, it is easy to find a nonregular digraph \( D \) with general adjacency matrix \( A_{\varphi} \) such that \( \sigma_1(A_{\varphi}) \neq 1 \). For instance, consider a \((r_1, r_2)\)-semi-regular graph \( G \) (i.e. a bipartite graph in which each vertex in the same partition has the same degree) with adjacency matrix \( A \). Then by (2) it is clear that \( A_{\varphi} = \varphi_{r_1 r_2} \). A. But it is well known that the spectral radius of \( G \) is \( \rho(A) = \sqrt{r_1 r_2} \) (see [7, p. 49]). Consequently, since \( A_{\varphi} \) is a symmetric matrix, \( \sigma_1(A_{\varphi}) = \rho(A_{\varphi}) = \sqrt{r_1 r_2} \neq 1 \), by choosing \( r_1, r_2 \) such that \( \frac{2\sqrt{r_1 r_2}}{r_1 + r_2} \neq 1 \).

Also, many of the relevant degree based topological indices \( \varphi \) (different from the general Randić index) do not satisfy the condition \( \text{rank}(A_{\varphi}) = \text{rank}(A) \), for all digraphs \( D \), as we can see next.

Example 2.6. Consider the digraph shown in Fig. 3. The Randić matrix of \( D \) is

\[
A_R = \begin{pmatrix}
0 & 1 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} \\
0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} & \frac{1}{2} & 0 \\
\frac{1}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} \\
\frac{1}{2\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{3}} & 0 \\
\frac{1}{2\sqrt{3}} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

and the adjacency matrix of \( D \) is

\[
A = \begin{pmatrix}
0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

Note that \( \text{rank}(A_{R_1}) = \text{rank}(A_{R_2}) = \text{rank}(A_{R_3}) = \text{rank}(A_{R_4}) = \text{rank}(A_{R_5}) = 5 \).

3. Upper and lower bounds for the Randić energy of digraphs

In this section, taking advantage of nice properties the Randić matrix has, we find upper and lower bounds for the Randić energy of digraphs.

The energy of a digraph \( D \) with respect to the Randić index \( R \), called Randić energy of \( D \) and denoted by \( E_R(D) \), is obtained from (3) by substituting \( \varphi \) by \( R \). In other words,

\[
E_R(D) = \sum_{i=1}^{n} \sigma_i(A_R),
\]

where

\[
\sigma_1(A_R) \geq \sigma_2(A_R) \geq \cdots \geq \sigma_n(A_R) \geq 0
\]

are singular values of \( A_R \). Note that (4) generalizes the concept of Randić energy of graphs introduced in [3].

Theorem 3.1. Let \( D \) be a digraph (with at least one arc). Then

\[
E_R(D) \geq 1.
\]

Moreover, \( E_R(D) = 1 \) if and only if \( D \) is a sink-source orientation of a complete bipartite graph.

Proof. Let \( A_R \) be the Randić matrix of \( D \). By Lemma 2.3, \( \sigma_1(A_R) = 1 \). Hence

\[
E_R(D) = \sum_{i=1}^{n} \sigma_i(A_R) \geq 1.
\]

For the second part, by (5) and Lemma 2.4, \( E_R(D) = 1 \) if and only if \( \text{rank}(D) = \text{rank}(A_R) = 1 \). It follows from [1, Corollary 3.11] that this occurs if and only if \( D \) is a sink-source orientation of a complete bipartite graph. \( \square \)
Next we find an upper bound for the Randić energy of a digraph in terms of its rank.

**Theorem 3.2.** Let $D$ be a digraph. Then

$$E_R(D) \leq \text{rank}(D).$$

Equality occurs if and only if $H_D$ is a disjoint union of complete bipartite graphs.

**Proof.** By Lemma 2.3 and Lemma 2.4, $\sigma_1(A_R) = 1$ and $\text{rank}(A_R) = \text{rank}(D)$. The result follows from [23, Thm. 4.5]. □

**Example 3.3.** Let us see some examples of digraphs which satisfy the equality condition of Theorem 3.2. Consider the digraphs $D_1$, $D_2$, and $D$ shown in Fig. 4. The characteristic polynomial of $A_R(D)\top A_R(D)$ is equal to $x_i(i-1)^3$, for $i = 1, 2, 3$. Then $E_R(D) = 3 = \text{rank}(D)$, for $i = 1, 2, 3$. Note that

- $H_{D_1} = K_{1,1} + K_{1,1} + K_{1,1}$
- $H_{D_2} = K_{1,1} + K_{1,2} + K_{1,2}$
- $H_{D_3} = K_{1,2} + K_{1,2} + K_{1,2}.$

Recall that a digraph is 1-regular if $d^+_{uv} = d^-_{uv} = 1$ for all vertex $u$ of $D$. One consequence of Theorem 3.2 is the next

**Corollary 3.4.** Let $D$ be a digraph with $n$ vertices. Then

$$E_R(D) \leq n.$$

Equality occurs if and only if $D$ is 1-regular.

**Proof.** By Theorem 3.2,

$$E_R(D) \leq \text{rank}(D) \leq n. \quad (6)$$

Assume that $E_R(D) = n$. Then by Lemma 2.3, $\sigma_1(A_R) = 1$ for $i = 1, \ldots, n$, and by (6), $\text{rank}(D) = n$. Now from the singular value decomposition theorem [14, Theorem 2.6.3], $A_R$ is unitary. Hence, for all $i = 1, \ldots, n$,

$$1 = \left|A_R A_R^\top \right|_{ii} = \sum_{j=1}^{n} |A_R|_{ij}^2 = \sum_{i,j \in E} \frac{1}{d_i} \sum_{v \in E} (d_i)^{-1} \frac{1}{d_j} = \frac{1}{d_i} \sum_{v \in E} \frac{1}{d_j} \frac{1}{d_i} = \frac{1}{d_i} d_i = 1. \quad (7)$$

Let $v_i$ be any vertex of $D$. Then $d^-_{v_i} > 0$, otherwise all entries of column $j$ of $A_R$ are equal to zero, which implies $\text{rank}(D) < n$, a contradiction. So there is a vertex $v_j$ such that $v_i v_j \in E(D)$. By (7), $d^-_{v_i} = 1$. Then all vertices of $D$ have indegree equal to 1. By a similar argument, all vertices of $D$ have outdegree equal to 1. Therefore, $D$ is 1-regular.

Conversely, if $D$ is 1-regular then $A(D) = A_R(D)$, consequently, $n = E(D) = E_R(D).$ □

In order to present a graph version of Theorem 3.2, we need to characterize graphs $G$ such that $H_G$ is a disjoint union of complete bipartite graphs. Recall that the direct product of graphs $G$ and $H$ is the graph $G \times H$, with vertex set $V(G) \times V(H)$, where the vertices $(a, b)$ and $(c, d)$ are adjacent if $ac \in E(G)$ and $bd \in E(H)$. It is known that the adjacency matrix of $G \times H$ is the Kronecker product of the adjacency matrix of $G$ and $H$, i.e., $A(G \times H) = A(G) \otimes A(H)$ [28].

**Remark 3.5.** If $G$ is a graph, then $H_G = K_2 \times G$, the direct product of the graphs $K_2$ and $G$. From well-known properties of the product of graphs [28], if $G$ is connected and not bipartite, then $H_G$ is connected. On the other hand, if $G$ is a connected bipartite graph, then $H_G = G + G$, the disjoint union of $G$ and $G$. For instance, if $k$ is a positive integer, $H_{C_{2k}} = C_{4k} + C_{4k}$, and $H_{K_{2k+1}} = C_{4k+2}$.

**Proposition 3.6.** Let $G$ be a connected graph. Then $H_G$ is a direct sum of complete bipartite graphs if and only if $G$ is a complete bipartite graph.

**Proof.** Assume that $H_G$ is a disjoint union of complete bipartite graphs. If $G$ is a bipartite graph then $H_G = G + G$, which implies that $G$ is a complete bipartite graph. Otherwise, $G$ is not bipartite, and so $H_G$ is connected. Hence $H_G = K_2 \times G$ is a complete bipartite graph. It follows that

$$2 = \text{rank}(A(K_2 \times G)) = \text{rank}(A(K_2) \otimes A(G)) = \frac{1}{2} \text{rank}(A(K_2))\text{rank}(A(G)) = 2\text{rank}(A(G)),$$

and so $\text{rank}(G) = 1$, a contradiction.

Conversely, if $G$ is a complete bipartite graph then $H_G = G + G$ is a disjoint union of complete bipartite graphs, where $G$ is the symmetric digraph associated to $G$ (i.e. each edge $uv$ of $G$ is substituted by a pair of arcs $uv$ and $vu$). □

In the general case of digraphs, the situation is more complicated, as we can see in the following example.

**Example 3.7.** All digraphs $D_1$, $D_2$ and $D_3$ in Fig. 5 satisfy

$$H_D = K_{2,1} + K_{2,1},$$

for each $i \in \{1, 2, 3\}$.

Now we can give the graph version of Theorem 3.2.

**Theorem 3.8.** Let $G$ be a graph. Then

$$E_R(G) \leq \text{rank}(G).$$

Moreover, $G$ is a disjoint union of complete bipartite graphs if and only if equality holds.

**Proof.** Direct consequence of Theorem 3.2 and Proposition 3.6. □

The Randić index $R(D)$ of a digraph $D$ is the case $a = -\frac{1}{2}$ in the general Randić index defined for any $a \in \mathbb{R}$ as $R_a(D) = \sum_{e \in E(D)} (d^+_e)^a$. In our next result we compare $E_R(D)$ with $R_{-1}(D)$. Note that there is a close relation between sums of the squares of the singular values of $A_R$, and the VDB topological index $R_{-1}(D)$:

$$\sum_{i=1}^{n} \sigma_i^2(A_R) = \text{tr}(A_R^\top A_R) = 2R_{-1}(D). \quad (8)$$
Theorem 3.9. Let $D$ be a digraph with $n$ vertices. Then
\[ 2R_{-1}(D) \leq E_R(D) \leq \sqrt{2n} \sqrt{R_{-1}(D)}. \]
Equality on the left occurs if and only if $H_D$ is a disjoint union of complete bipartite graphs. Equality on the right occurs if and only if $D$ is 1-regular.

Proof. Consider the vectors $(1, \ldots, 1)$ and $(\sigma_1(A_R), \sigma_2(A_R), \ldots, \sigma_n(A_R))$ of $\mathbb{R}^n$. By Cauchy-Schwarz inequality and relation (8), we deduce that
\[ E_R(D) = \sum_{i=1}^n \sigma_i(A_R) \leq \sqrt{n} \sqrt{\sum_{i=1}^n \sigma_i^2(A_R)} = \sqrt{2n} \sqrt{R_{-1}(D)}. \]
(9)

Now assume that $E_R(D) = \sqrt{2n} \sqrt{R_{-1}(D)}$. Then by (9) and Lemma 2.3, $\sigma_i(A_R) = 1$ for all $i$ and so $E_R(D) = n$. It results from Corollary 3.4 that $D$ is 1-regular.

Conversely, assume that $D$ is 1-regular. Then clearly $A_R = A$ and $E_R(D) = E(D) = n$. On the other hand, let
\[ \sqrt{2n} \sqrt{R_{-1}(D)} = \sum_{i=1}^n \frac{1}{d_U d_V} = \sqrt{n}. \]
To see the inequality on the left, note that by Lemma 2.3, $\sigma_i(A_R) \leq 1$ for all $i$. Hence
\[ E_R(D) = \sum_{i=1}^n \sigma_i(A_R) \geq \sum_{i=1}^n \sigma_i^2(A_R) = 2R_{-1}(D). \]
(10)

Note that by (10), $E_R(D) = 2R_{-1}(D)$ if and only if
\[ \sum_{i=1}^n \sigma_i(A_R) = \sum_{i=1}^n \sigma_i^2(A_R). \]
or equivalently,
\[ \sum_{i=1}^n \sigma_i(A_R) (1 - \sigma_i(A_R)) = 0. \]
(11)

Since $0 \leq \sigma_i(A_R) \leq 1$ for all $i$ (see Lemma 2.3), clearly (11) occurs if and only if
\[ \sigma_i(A_R) = 1 \quad \text{or} \quad \sigma_i(A_R) = 0, \]
for all $i = 1, \ldots, n$. By Lemma 2.4 and the fact that the number of nonzero singular values of $A_R$ is precisely $\text{rank}(A_R)$, we deduce that (12) occurs if and only if
\[ E_R(D) = \sum_{i=1}^n \sigma_i(A_R) = \text{rank}(A_R) = \text{rank}(D). \]

and, by Theorem 3.2, this occurs if and only if $H_D$ is a disjoint union of complete bipartite graphs. \hfill $\square$

We can go further and find upper and lower bounds of the Randić energy in terms of invariants of the digraph. Let $p$ be the number of sink vertices of $D$ and $q$ the number of source vertices of $D$. Furthermore, let
\[ \delta^+ = \min_{d^+ > 0} \left\{ d^+_u \right\}, \quad \delta^- = \min_{d^- > 0} \left\{ d^-_v \right\}, \quad \Delta^+ = \max_{u \in V} \left\{ d^+_u \right\}, \quad \Delta^- = \max_{v \in V} \left\{ d^-_v \right\}. \]

Moreover, let
\[ \Delta = \max \left\{ \Delta^+, \Delta^- \right\}. \]

Theorem 3.10. Let $D$ be a digraph with $n$ vertices. Then
\[ \frac{2n - (p + q)}{2\Delta} \leq E_R(D) \leq \sqrt{\frac{n}{2} \left( (n - p) \frac{1}{\delta^+} + (n - q) \frac{1}{\delta^-} \right)} \]
Equality on the left occurs if and only if $H_D$ is a disjoint union of complete bipartite graphs of the form $K_{\Delta^+, \Delta^-}$. Equality on the right occurs if and only if $D$ is 1-regular.

Proof. Any real numbers $x, y$ satisfy
\[ xy \leq \frac{1}{2} \left( x^2 + y^2 \right), \]
where equality occurs if and only if $x = y$. Hence
\[ 2R_{-1}(D) = \sum_{u \in E} \frac{1}{d^+_u d^-_v} \geq \frac{1}{2} \sum_{u \in E} \left( \frac{1}{(d^+_u)^2} + \frac{1}{(d^-_v)^2} \right) \]
\[ = \frac{1}{2} \left( \sum_{d^+_u > 0} \frac{1}{d^+_u} + \sum_{d^-_v > 0} \frac{1}{d^-_v} \right) \]
\[ \leq \frac{1}{2} \left( (n - p) \frac{1}{\delta^+} + (n - q) \frac{1}{\delta^-} \right). \]
From Theorem 3.9 we obtain
\[ E_R(D) \leq \sqrt{2nR_{-1}(D)} \leq \sqrt{\frac{n}{2} \left( (n - p) \frac{1}{\delta^+} + (n - q) \frac{1}{\delta^-} \right)} . \]
(13)

If $E_R(D) = \sqrt{2nR_{-1}(D)}$, then, by (13), $E_R(D) = \sqrt{2nR_{-1}(D)}$, and by Theorem 3.9, $D$ is 1-regular.

Conversely, if $D$ is 1-regular then, $p = q = 0$ and $\delta^+ = \delta^- = 1$, consequently
\[ \sqrt{\frac{n}{2} \left( (n - p) \frac{1}{\delta^+} + (n - q) \frac{1}{\delta^-} \right)} = \sqrt{n} \frac{n}{2} = n = E_R(D). \]

The other inequality comes from the fact that
\[ 2R_{-1}(D) = \sum_{u \in E} \frac{1}{d^+_u d^-_v} \geq \sum_{u \in E} \frac{1}{(d^-_v)^2} = \frac{1}{\Delta} \sum_{d^-_v > 0} d^-_v \]
\[ = \frac{1}{\Delta} (n - q) \geq \frac{1}{\Delta} (n - q) \leq \frac{1}{\Delta} (n - p) \leq \frac{1}{\Delta} (n - p). \]
(14)

Similarly,
\[ 2R_{-1}(D) = \sum_{u \in E} \frac{1}{d^+_u d^-_v} \geq \sum_{u \in E} \frac{1}{(d^+_u)^2} = \frac{1}{\Delta} \sum_{d^+_u > 0} d^+_u \]
\[ = \frac{1}{\Delta} (n - p) \geq \frac{1}{\Delta} (n - p) \geq \frac{1}{\Delta} (n - p). \]
(15)

It follows from (14), (15) and Theorem 3.9 that
\[ E_R(D) \geq 2R_{-1}(D) \geq \frac{2n - (p + q)}{2\Delta}. \]
(16)

If $E_R(D) = \frac{2n - (p + q)}{2\Delta}$, then, by (16), $E_R(D) = 2R_{-1}(D)$ which is equivalent by Theorem 3.9 to say that $H_D$ is a disjoint union of complete bipartite graphs. Therefore, $S_D$ is a disjoint union of sink-source orientations of complete bipartite graphs. On the other hand, by (14) and (15), for all $uv \in E(D)$,
\[ d^+_u = d^-_v = \Delta. \]
This clearly implies that every sink vertex or source vertex in $S_D$ has in-degree or out-degree equal to $\Delta$, respectively. Hence $H_D$ is a disjoint union of complete bipartite graphs of the form $K_{\Delta, \Delta}$. Conversely, assume that $D$ is a digraph such that $H_D$ is a disjoint union of $k$ complete bipartite graphs of the form $K_{\Delta, \Delta}$. Then $S_D$ is a disjoint union of $k$ sink-source orientations of $K_{\Delta, \Delta}$. In particular,

$$E_R(D) = E_R(S_D) = k = \frac{n(S_D)}{2\Delta}. \tag{17}$$

Let $s$ be the number of splitting vertices of $D$. Then

$$n(S_D) = 2s + p + q = 2(n - p - q) + p + q = 2n - (p + q). \tag{18}$$

It follows from (17) and (18) that $E_R(D) = \frac{2n-(p+q)}{2\Delta}$. □

4. Concluding remarks

Among all general adjacency matrices associated to a VDB topological index, the Randić matrix $A_R$ is distinguished by its algebraic properties, namely, its spectral norm is equal to 1 and its rank coincides with the adjacency matrix. Based on these properties, we can obtain upper and lower bounds for the Randić energy of digraphs. Some of these bounds generalize known results for the Randić energy of graphs, thus our results provide a new perspective from a more general point of view. But also, we deduce new results on the Randić energy of graphs as particular cases. For instance, $E_R(G) \leq \text{rank}(G)$ for all graphs $G$. Moreover, equality occurs if and only if $G$ is a disjoint union of complete bipartite graphs.

In our opinion, this is just the beginning of research on energy associated to a VDB topological index over digraphs. Recall that graphs and symmetric digraphs are in one to one correspondence, by identifying an edge of the graph with a pair of symmetric arcs in the digraph. So the class of digraphs is an extremely large class which includes non-symmetric digraphs, used to represent real-world situations such as social networks, transportation networks, chemical and biological networks, etc.

The generalization of VDB topological indices and its associated energy to digraphs opens innumerable directions in research. For instance, given a significant class of digraphs $D$, find upper and lower bounds of $E_R$ over $D$ in terms of certain parameters of the digraph (such as number of vertices or number of arcs). Also, the extremal value problem of $E_R$ over $D$ is of great interest in spectral (di)graph theory. For example, given a graph (or set of graphs), consider the problem of finding extremal values of $E_R$ among all orientations of the graph (or set of graphs). On the other hand, based on known results from graph energy associated to a VDB topological index, it is natural to investigate how these can be extended to digraphs.

Declarations

Author contribution statement

Juan Rada, Roberto Cruz, Juan Monsalve: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data; Wrote the paper.

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