Heliyon 8 (2022) e11874

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Research article

Randić energy of digraphs

Roberto Cruz, Juan Monsalve, Juan Rada *

Instituto de Matemáticas, Universidad de Antioquia, Medellín, Colombia

ARTICLE INFO

Keywords:
Randić energy
Randić index
VDB topological index
Digraphs

ABSTRACT

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

$$\varphi(D)=\frac{1}{2}\sum_{uv\in E(D)}\varphi_{d_u^+,d_v^-},$$

where d_u^+ and d_v^- 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 $[A_\varphi]_{ij}=\varphi_{d_{v_i}^+,d_{v_j}^-}$ if $v_iv_j\in E(D)$, and 0 otherwise. The energy of D with respect to a VDB index φ is defined as $\mathcal{E}_\varphi(D)=\sum_{i=1}^n\sigma_i(A_\varphi)$, where $\sigma_1(A_\varphi)\geq\sigma_2(A_\varphi)\geq\cdots\geq\sigma_n(A_\varphi)\geq 0$ are the singular values of the matrix A_φ.

We will show that in case $\varphi=\mathcal{R}$ is the Randić index, the spectral norm of $A_\mathcal{R}$ is equal to 1, and rank of $A_\mathcal{R}$ 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 $\mathcal{E}_\mathcal{R}$ 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 $\mathcal{E}_\mathcal{R}(G)\leq rank(G)$ 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 and arc sets denoted by $V=V(D)$ 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 $d_u^-=|\{vu\in E(D):v\in V(D)\}|$ (resp. outdegree $d_u^+=|\{uv\in E(D):v\in V(D)\}|$). 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

$$\varphi(D)=\frac{1}{2}\sum_{uv\in E(D)}\varphi_{d_u^+,d_v^-}, \tag{1}$$

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

$$[A_\varphi]_{ij}=\begin{cases}\varphi_{d_{v_i}^+,d_{v_j}^-} & \text{if } v_iv_j\in E(D)\\ 0 & \text{otherwise.}\end{cases} \tag{2}$$

In [23] the concept of energy of D with respect to φ was introduced as

$$\mathcal{E}_\varphi(D)=\sum_{i=1}^n\sigma_i(A_\varphi), \tag{3}$$

where

$$\sigma_1(A_\varphi)\geq\sigma_2(A_\varphi)\geq\cdots\geq\sigma_n(A_\varphi)\geq 0$$

* Corresponding author.
E-mail address: pablo.rada@udea.edu.co (J. Rada).

https://doi.org/10.1016/j.heliyon.2022.e11874
Received 17 June 2022; Received in revised form 31 August 2022; Accepted 17 November 2022

2405-8440/© 2022 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

are the singular values of the matrix A_φ (i.e. positive square roots of eigenvalues of $A_\varphi A_\varphi^\top$). In case $\varphi_{i,j} \equiv 1$, A_φ coincides with the usual adjacency matrix A of D, and $\mathcal{E}_\varphi(D)$ reduces to the energy $\mathcal{E}(D) = \sum_{i=1}^n \sigma_i(A)$. Recall that $\mathcal{E}(D)$ 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 $\mathcal{E}(G) = \sum_{i=1}^n |\lambda_i|$ [10, 17]. Note that in this case, the eigenvalues of $AA^\top = A^2$ 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 φ, 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 $\mathcal{R}$. 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 $\mathcal{E}_\varphi$ just started in [23]. Naturally, innumerable problems arise in the study of $\mathcal{E}_\varphi$ 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 in this paper to the Randić energy of digraphs. It comes out that the Randić matrix $A_\mathcal{R}$ of a digraph D has remarkable properties, namely, the spectral norm of $A_\mathcal{R}$ is equal to 1, and rank of $A_\mathcal{R}$ 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 $\mathcal{E}_\mathcal{R}$ 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 $\mathcal{E}_\mathcal{R}(G) \le rank(G)$ 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 $\varphi_{i,j}$ by $\frac{1}{\sqrt{ij}}$ in (1) we obtain the Randić index of a digraph D:

$$\mathcal{R} = \mathcal{R}(D) = \frac{1}{2} \sum_{uv \in E(D)} \frac{1}{\sqrt{d_u^+ \cdot d_v^-}}.$$

In this case, the general adjacency matrix $A_\mathcal{R}$ of D is called Randić matrix of D, and it is defined as

$$\left[A_\mathcal{R}\right]_{ij} = \begin{cases} \frac{1}{\sqrt{d_{v_i}^+ d_{v_j}^-}} & \text{if } v_i v_j \in E(D) \\ 0 & \text{otherwise.} \end{cases}$$

In order to study the Randić matrix $A_\mathcal{R}$, let us recall the concept of splitting digraph [23]. Let D be a digraph and consider the set

$$T = \left\{u \in V(D) : d_u^+ \neq 0\right\}$$

of *tails* of D and the set

$$H = \left\{u \in V(D) : d_u^- \neq 0\right\}$$

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

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

The arc set of S_D is given by $E\left(S_D\right) = \left\{u^t v^h : uv \in E\right\}$. 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 $T = \left\{u_1, u_3\right\}$, and the set of heads of Q is $H = \left\{u_2, u_3\right\}$. Then the vertex set of S_Q is

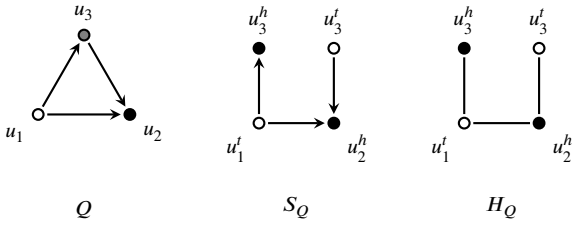

Fig. 1. Digraph Q, its splitting digraph S_Q and its underlying graph H_Q in Example 2.1.

$$V\left(S_Q\right) = \{u_1^t, u_3^t, u_2^h, u_3^h\}$$

and

$$E\left(S_Q\right) = \{u_1^t u_2^h, u_1^t u_3^h, u_3^t u_2^h\}$$

is the arc set of S_Q (see Fig. 1).

Example 2.2. Consider the digraph D depicted in Fig. 2. In this case, the set of tails of D is $T = \{b, c, d, e, f, g\}$, and the set of heads of Q is $H = \{a, b, c, e, f, g\}$. Hence

$$V(S_D) = \left\{b^t, c^t, d^t, e^t, f^t, g^t, a^h, b^h, c^h, e^h, f^h, g^h\right\},$$

and

$$E(S_D) = \left\{b^t a^h, c^t b^h, c^t f^h, d^t c^h, d^t e^h, d^t g^h, e^t a^h, f^t a^h, g^t b^h, g^t f^h\right\}.$$

The representation of S_D and its underlying graph H_D 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 $A_\mathcal{R}$ has.

Lemma 2.3. *Let D be a digraph (with at least one arc) and Randić matrix $A_\mathcal{R}$. Then $\sigma_1\left(A_\mathcal{R}\right) = 1$.*

Proof. By [20, Theorem 2.1], the spectral radius of the matrix $A_\mathcal{R}\left(H_D\right)$ is $\rho\left(A_\mathcal{R}\left(H_D\right)\right) = 1$. It follows from [23, Lemma 3.2] that

$$\sigma_1\left(A_\mathcal{R}\right) = \rho\left(A_\mathcal{R}\left(H_D\right)\right) = 1. \quad \square$$

On the other hand, recall that the rank of a digraph D is the rank of the adjacency matrix A of D. Namely,

$$rank\,(D) = rank\,(A).$$

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 $rank\left(A_\mathcal{R}\right) = rank(D)$.*

Proof. Given a n-vertex digraph Ds, let D^+ (resp. D^-) be the $n \times n$ diagonal matrix whose j-th diagonal entry is $\max\left\{1, d_j^+\right\}$ (resp. $\max\left\{1, d_j^-\right\}$). By direct matrix multiplication we can see that

$$A_\mathcal{R} = \left(D^+\right)^{-1/2} A \left(D^-\right)^{-1/2}.$$

Since the matrices D^+ and D^- are nonsingular, and multiplying by a nonsingular matrix does not change the rank of A, it follows

$$rank(A_\mathcal{R}) = rank(A) = rank(D). \quad \square$$

We are interested in those VDB topological indices φ such that $\sigma_1(A_\varphi) = 1$ and $rank(A_\varphi) = rank(A)$, for all digraphs D. Certainly, the Randić index $\mathcal{R}$ is one of them. The general Randić index $\mathcal{R}_\alpha$ is obtained

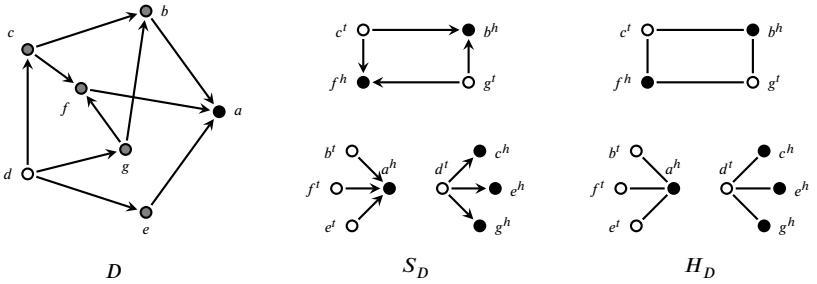

Fig. 2. The digraph D, the splitting digraph S_D, and underlying graph H_D.

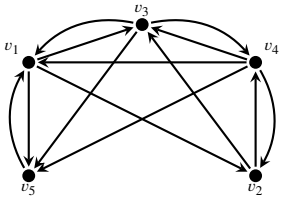

Fig. 3. The digraph D used in Example 2.6.

from the function $\varphi_{i,j} = (ij)^\alpha$, where $\alpha \in \mathbb{R}$. In particular, $\mathcal{R} = \mathcal{R}_{-\frac{1}{2}}$. A similar proof to the proof of Lemma 2.4 shows that $rank(A_{\mathcal{R}_\alpha}) = rank(A)$, for all $\alpha \in \mathbb{R}$. However, the only value for which $\sigma_1(A_{\mathcal{R}_\alpha}) = 1$ is $\alpha = -\frac{1}{2}$, as we shall see in our next example.

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

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

The Harmonic index, induced by the function $\varphi_{i,j} = \frac{2}{i+j}$, is an exception since $r\varphi_{r,r} = 1$. However, it is easy to find a nonregular digraph D with general adjacency matrix A_φ such that $\sigma_1(A_\varphi) \neq 1$. For instance, consider a (r_1, r_2)-semiregular 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_φ is a symmetric matrix, $\sigma_1(A_\varphi) = \rho(A_\varphi) = \sqrt{r_1 r_2}\varphi_{r_1 r_2} \neq 1$, 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 φ (different from the general Randić index) do not satisfy the condition $rank(A\varphi) = rank(A)$, 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

$$A_{\mathcal{R}} = \begin{pmatrix} 0 & \frac{1}{\sqrt{6}} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{2} & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{3} \\ \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{3}} & 0 & \frac{1}{2\sqrt{3}} \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \end{pmatrix}$$

and the adjacency matrix of D is

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

Note that $rank\left(A_{\mathcal{R}}\right) = rank(D) = rank(A) = 4$. However,

$$rank(A_{\mathcal{FZ}}) = rank(A_{\mathcal{H}}) = rank(A_{\mathcal{SC}}) = rank(A_{\mathcal{SO}}) = rank(A_{\mathcal{F}}) = rank(A_{\mathcal{GA}}) = rank(A_{\mathcal{ISI}}) = 5,$$

where $A_{\mathcal{FZ}}$ is the First Zagreb matrix of D with $\varphi_{i,j} = i + j$; $A_{\mathcal{H}}$ is the Harmonic matrix of D with $\varphi_{i,j} = 2/(i+j)$; $A_{\mathcal{SC}}$ is the Sum-Connectivity matrix of D with $\varphi_{i,j} = 1/\sqrt{i+j}$; $A_{\mathcal{SO}}$ is the Sombor matrix of D with $\varphi_{i,j} = \sqrt{i^2 + j^2}$; $A_{\mathcal{F}}$ is the Forgotten matrix of D with $\varphi_{i,j} = i^2 + j^2$; $A_{\mathcal{GA}}$ is the Geometric-Arithmetic matrix of D with $\varphi_{i,j} = (2\sqrt{ij})/(i+j)$ and A_{ISI} is the Inverse Sum Indeg matrix of D with $\varphi_{i,j} = (ij)/(i+j)$.

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 $\mathcal{R}$, called Randić energy of D and denoted by $\mathcal{E}_{\mathcal{R}}(D)$, is obtained from (3) by substituting φ by $\mathcal{R}$. In other words,

$$\mathcal{E}_{\mathcal{R}}(D) = \sum_{k=1}^{n} \sigma_k(A_{\mathcal{R}}), \tag{4}$$

where

$$\sigma_1\left(A_{\mathcal{R}}\right) \geq \sigma_2\left(A_{\mathcal{R}}\right) \geq \cdots \geq \sigma_n\left(A_{\mathcal{R}}\right) \geq 0$$

are singular values of $A_{\mathcal{R}}$. 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*

$$\mathcal{E}_{\mathcal{R}}(D) \geq 1.$$

Moreover, $\mathcal{E}_{\mathcal{R}}(D) = 1$ if and only if D is a sink-source orientation of a complete bipartite graph.

Proof. Let $A_{\mathcal{R}}$ be the Randić matrix of D. By Lemma 2.3, $\sigma_1\left(A_{\mathcal{R}}\right) = 1$. Hence

$$\mathcal{E}_{\mathcal{R}}(D) = \sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}}) \geq 1. \tag{5}$$

For the second part, by (5) and Lemma 2.4, $\mathcal{E}_{\mathcal{R}}(D) = 1$ if and only if $rank(D) = rank\left(A_{\mathcal{R}}\right) = 1$. 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. □

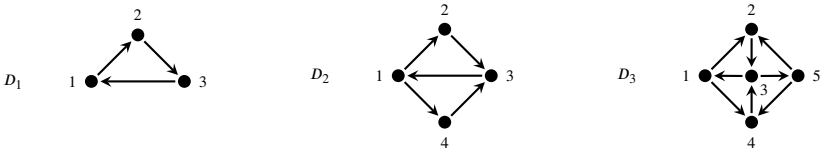

Fig. 4. Digraphs D_1, D_2 and D_3 which satisfy the equality condition in Theorem 3.2.

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*

$$\mathcal{E}_{\mathcal{R}}(D) \leqslant rank(D).$$

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, $\sigma_1(A_{\mathcal{R}}) = 1$ and $rank(A_{\mathcal{R}}) = rank(D)$. 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_3 shown in Fig. 4. The characteristic polynomial of $A_{\mathcal{R}}(D_i)^{\top} A_{\mathcal{R}}(D_i)$ is equal to $\lambda^{i-1}(\lambda-1)^3$, for $i = 1, 2, 3$. Then $\mathcal{E}_{\mathcal{R}}(D_i) = 3 = rank(D_i)$, for $i = 1, 2, 3$. Note that

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

Recall that a digraph is 1-regular if $d_u^+ = d_u^- = 1$ 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*

$$\mathcal{E}_{\mathcal{R}}(D) \leqslant n.$$

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

Proof. By Theorem 3.2,

$$\mathcal{E}_{\mathcal{R}}(D) \leqslant rank(D) \leq n. \tag{6}$$

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

$$1 = \left[A_{\mathcal{R}} A_{\mathcal{R}}^{\top}\right]_{ii} = \sum_{j=1}^{n} \left[A_{\mathcal{R}}\right]_{ij}^2 = \sum_{v_i v_j \in E} \frac{1}{d_{v_i}^+ d_{v_j}^-} = \frac{1}{d_{v_i}^+} \sum_{v_i v_j \in E} \frac{1}{d_{v_j}^-} \leq \frac{1}{d_{v_i}^+} d_{v_i}^+ = 1. \tag{7}$$

Let v_j be any vertex of D. Then $d_{v_j}^- > 0$, otherwise all entries of column j of $A_{\mathcal{R}}$ are equal to zero, which implies $rank(D) < n$, a contradiction. So there is a vertex v_i such that $v_i v_j \in E(D)$. By (7), $d_{v_j}^- = 1$. 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 $A(D) = A_{\mathcal{R}}(D)$, consequently,

$$n = \mathcal{E}(D) = \mathcal{E}_{\mathcal{R}}(D). \quad \square$$

In order to present a graph version of Theorem 3.2, we need to characterize graphs G such that $H_{\widehat{G}}$ 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 $H_{\widehat{G}} = K_2 \times G$, the direct product of the graphs K_2 and G. From well known properties of direct product of graphs [28], if G is connected and not bipartite, then $H_{\widehat{G}}$ is connected. On the other hand, if G is a connected bipartite graph, then $H_{\widehat{G}} = G + G$, the disjoint union of G and G. For instance, if k is a positive integer, $H_{\widehat{C}_{2k}} = C_{2k} + C_{2k}$ and $H_{\widehat{C}_{2k+1}} = C_{4k+2}$.

Proposition 3.6. *Let G be a connected graph. Then $H_{\widehat{G}}$ is a direct sum of complete bipartite graphs if and only if G is a complete bipartite graph.*

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

$$2 = rank\left(A(K_2 \times G)\right) = rank\left(A(K_2) \otimes A(G)\right)$$
$$= rank\left(A(K_2)\right) rank\left(A(G)\right) = 2 rank\left(A(G)\right),$$

and so $rank(G) = 1$, a contradiction.

Conversely, if G is a complete bipartite graph then $H_{\widehat{G}} = G + G$ is a disjoint union of complete bipartite graphs, where $\widehat{G}$ 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

$$H_{D_i} = K_{2,1} + K_{2,1},$$

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*

$$\mathcal{E}_{\mathcal{R}}(G) \leq rank(G).$$

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 $\mathcal{R}(D)$ of a digraph D is the case $\alpha = -\frac{1}{2}$ in the general Randić index defined for any $\alpha \in \mathbb{R}$ as $\mathcal{R}_\alpha(D) = \sum_{uv \in E(D)} \left(d_u^+ d_v^-\right)^\alpha$. In our next result we compare $\mathcal{E}_{\mathcal{R}}(D)$ with $\mathcal{R}_{-1}(D)$. Note that there is a close relation between sums of the squares of the singular values of $A_{\mathcal{R}}$, and the VDB topological index $\mathcal{R}_{-1}(D)$:

$$\sum_{i=1}^{n} \sigma_i^2\left(A_{\mathcal{R}}\right) = tr\left(A_{\mathcal{R}}^{\mathrm{T}} A_{\mathcal{R}}\right) = 2\mathcal{R}_{-1}(D). \tag{8}$$

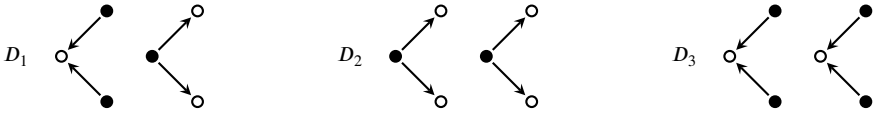

Fig. 5. Digraphs D_1, D_2 and D_3, such that H_{D_i} is a disjoint union of complete bipartite graphs for each $i \in \{1,2,3\}$.

Theorem 3.9. *Let D be a digraph with n vertices. Then*

$$2\mathcal{R}_{-1}(D) \leq \mathcal{E}_{\mathcal{R}}(D) \leq \sqrt{2n\mathcal{R}_{-1}(D)}.$$

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 $\left(\sigma_1(A_{\mathcal{R}}), \sigma_2(A_{\mathcal{R}}), \ldots, \sigma_n(A_{\mathcal{R}})\right)$ of $\mathbb{R}^n$. By Cauchy-Schwarz inequality and relation (8), we deduce that

$$\mathcal{E}_{\mathcal{R}}(D) = \sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}}) \leq \sqrt{n}\sqrt{\sum_{i=1}^{n} \sigma_i^2(A_{\mathcal{R}})} = \sqrt{2n\mathcal{R}_{-1}(D)}. \tag{9}$$

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

Conversely, assume that D is 1-regular. Then clearly $A_{\mathcal{R}} = A$ and $\mathcal{E}_{\mathcal{R}}(D) = \mathcal{E}(D) = n$. On the other hand,

$$\sqrt{2n\mathcal{R}_{-1}(D)} = \sqrt{n\sum_{uv\in E} \frac{1}{d_u^+ d_v^-}} = \sqrt{n^2} = n.$$

To see the inequality on the left, note that by Lemma 2.3, $\sigma_i(A_{\mathcal{R}}) \leq 1$ for all i. Hence

$$\mathcal{E}_{\mathcal{R}}(D) = \sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}}) \geq \sum_{i=1}^{n} \sigma_i^2(A_{\mathcal{R}}) = 2\mathcal{R}_{-1}(D). \tag{10}$$

Note that by (10), $\mathcal{E}_{\mathcal{R}}(D) = 2\mathcal{R}_{-1}(D)$ if and only if

$$\sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}}) = \sum_{i=1}^{n} \sigma_i^2(A_{\mathcal{R}}),$$

or equivalently,

$$\sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}})\left(1 - \sigma_i(A_{\mathcal{R}})\right) = 0. \tag{11}$$

Since $0 \leqslant \sigma_i(A_{\mathcal{R}}) \leqslant 1$ for all i (see Lemma 2.3), clearly (11) occurs if and only if

$$\sigma_i(A_{\mathcal{R}}) = 1 \quad \text{or} \quad \sigma_i(A_{\mathcal{R}}) = 0, \tag{12}$$

for all $i = 1,\ldots,n$. By Lemma 2.4 and the fact that the number of nonzero singular values of $A_{\mathcal{R}}$ is precisely $rank(A_{\mathcal{R}})$, we deduce that (12) occurs if and only if

$$\mathcal{E}_{\mathcal{R}}(D) = \sum_{i=1}^{n} \sigma_i(A_{\mathcal{R}}) = rank(A_{\mathcal{R}}) = rank(D),$$

and, by Theorem 3.2, this occurs if and only if H_D is a disjoint union of complete bipartite graphs. □

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

$$\delta^+ = \min_{\substack{u\in V\\ d_u^+>0}}\left\{d_u^+\right\},\ \delta^- = \min_{\substack{u\in V\\ d_u^->0}}\left\{d_u^-\right\},\ \Delta^+ = \max_{u\in V}\left\{d_u^+\right\},\ \text{and}\ \Delta^- = \max_{u\in V}\left\{d_u^-\right\}.$$

Moreover, let

$$\Delta = \max\left\{\Delta^+, \Delta^-\right\}.$$

Theorem 3.10. *Let D be a digraph with n vertices. Then*

$$\frac{2n-(p+q)}{2\Delta} \leq \mathcal{E}_{\mathcal{R}}(D) \leq \sqrt{\frac{n}{2}\left((n-p)\frac{1}{\delta^+} + (n-q)\frac{1}{\delta^-}\right)}.$$

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

$$\begin{aligned} 2\mathcal{R}_{-1}(D) &= \sum_{uv\in E} \frac{1}{d_u^+ d_v^-} \leq \frac{1}{2}\sum_{uv\in E}\left(\frac{1}{\left(d_u^+\right)^2} + \frac{1}{\left(d_v^-\right)^2}\right) \\ &= \frac{1}{2}\left(\sum_{\substack{u\in V\\ d_u^+>0}} \frac{1}{d_u^+} + \sum_{\substack{v\in V\\ d_v^->0}} \frac{1}{d_v^-}\right) \\ &\leq \frac{1}{2}\left((n-p)\frac{1}{\delta^+} + (n-q)\frac{1}{\delta^-}\right). \end{aligned}$$

From Theorem 3.9 we obtain

$$\mathcal{E}_{\mathcal{R}}(D) \leq \sqrt{2n\mathcal{R}_{-1}(D)} \leq \sqrt{\frac{n}{2}\left((n-p)\frac{1}{\delta^+} + (n-q)\frac{1}{\delta^-}\right)}. \tag{13}$$

If $\mathcal{E}_{\mathcal{R}}(D) = \sqrt{\frac{n}{2}\left((n-p)\frac{1}{\delta^+} + (n-q)\frac{1}{\delta^-}\right)}$ then, by (13), $\mathcal{E}_{\mathcal{R}}(D) = \sqrt{2n\mathcal{R}_{-1}(D)}$, and by Theorem 3.9, D is 1-regular.

Conversely, if D is 1-regular then, $p = q = 0$ and $\delta^+ = \delta^- = 1$, consequently

$$\sqrt{\frac{n}{2}\left((n-p)\frac{1}{\delta^+} + (n-q)\frac{1}{\delta^-}\right)} = \sqrt{\frac{n}{2}(n+n)} = n = \mathcal{E}_{\mathcal{R}}(D).$$

The other inequality comes from the fact that

$$\begin{aligned} 2\mathcal{R}_{-1}(D) &= \sum_{uv\in E} \frac{1}{d_u^+ d_v^-} \geq \sum_{uv\in E} \frac{1}{(\Delta^+) d_v^-} = \frac{1}{\Delta^+}\sum_{\substack{v\in V\\ d_v^->0}} \frac{d_v^-}{d_v^-} \\ &= \frac{1}{\Delta^+}(n-q) \geq \frac{1}{\Delta}(n-q). \end{aligned} \tag{14}$$

Similarly,

$$\begin{aligned} 2\mathcal{R}_{-1}(D) &= \sum_{uv\in E} \frac{1}{d_u^+ d_v^-} \geq \sum_{uv\in E} \frac{1}{(\Delta^-) d_u^+} = \frac{1}{\Delta^-}\sum_{\substack{u\in V\\ d_u^+>0}} \frac{d_u^+}{d_u^+} \\ &= \frac{1}{\Delta^-}(n-p) \geq \frac{1}{\Delta}(n-p). \end{aligned} \tag{15}$$

It follows from (14), (15) and Theorem 3.9 that

$$\mathcal{E}_{\mathcal{R}}(D) \geq 2\mathcal{R}_{-1}(D) \geq \frac{2n-(p+q)}{2\Delta}. \tag{16}$$

If $\mathcal{E}_{\mathcal{R}}(D) = \frac{2n-(p+q)}{2\Delta}$ then, by (16), $\mathcal{E}_{\mathcal{R}}(D) = 2\mathcal{R}_{-1}(D)$ 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 Δ, 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,

$$\mathcal{E}_{\mathcal{R}}(D) = \mathcal{E}_{\mathcal{R}}\left(S_D\right) = k = \frac{n\left(S_D\right)}{2\Delta}. \tag{17}$$

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

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

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

4. Concluding remarks

Among all general adjacency matrices associated to a VDB topological index, the Randić matrix $A_{\mathcal{R}}$ 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, $\mathcal{E}_{\mathcal{R}}(G) \leq rank(G)$ 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 $\mathcal{D}$, find upper and lower bounds of $\mathcal{E}_{\varphi}$ over $\mathcal{D}$ in terms of certain parameters of the digraph (such as number of vertices or number of arcs). Also, the extremal value problem of $\mathcal{E}_{\varphi}$ over $\mathcal{D}$ is of great interest in spectral (di)graph theory. For example, given a graph (or set of graphs), consider the problem of finding extremal value of $\mathcal{E}_{\varphi}$ 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.

Funding statement

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Data availability statement

No data was used for the research described in the article.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

References

[1] N. Agudelo, J. Monsalve, J. Rada, On the characterization of digraphs with given rank, Linear Algebra Appl. 587 (2020) 215–227.
[2] S. Alikhani, N. Ghanbari, Randić energy of specific graphs, Appl. Math. Comput. 269 (2015) 722–730.
[3] Ş. Bozkurt, A.D. Güngör, I. Gutman, A.S. Çevik, Randić matrix and Randić energy, MATCH Commun. Math. Comput. Chem. 64 (2010) 239–250.
[4] Ş. Bozkurt, A.D. Güngör, I. Gutman, Randić spectral radius and Randić energy, MATCH Commun. Math. Comput. Chem. 64 (2010) 321–334.
[5] R.A. Brualdi, Spectra of digraphs, Linear Algebra Appl. 432 (2010) 2181–2213.
[6] M. Cavers, S. Fallat, S. Kirkland, On the normalized Laplacian energy and general Randíc index R_{-1} of graphs, Linear Algebra Appl. 433 (2010) 172–190.
[7] D.M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs, Academic Press, New York, San Francisco, London, 1980; VEB Deutscher Verlag der Wissenschaften, Berlin, 1980, 2nd ed., 1982.
[8] K.C. Das, S. Sun, I. Gutman, Normalized Laplacian eigenvalues and Randić energy of graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 45–59.
[9] K.C. Das, I. Gutman, I. Milovanović, E. Milovanović, B. Furtula, Degree-based energies of graphs, Linear Algebra Appl. 554 (2018) 185–204.
[10] I. Gutman, The energy of a graph, Ber. Math. Statist. Sekt. Forchungsz. Graz 103 (1978) 1–12.
[11] I. Gutman, B. Furtula, Ş. Bozkurt, On Randić energy, Linear Algebra Appl. 442 (2014) 50–57.
[12] I. Gutman, Relating graph energy with vertex-degree-based energies, Mil. Tech. Cour. 68 (2020) 715–725.
[13] I. Gutman, J. Monsalve, J. Rada, A relation between a vertex-degree-based topological index and its energy, Linear Algebra Appl. 636 (2022) 134–142.
[14] R. Horn, C. Johnson, Matrix Analysis, Cambridge University Press, Cambridge, 2013.
[15] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
[16] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure–Activity Analysis, Wiley, New York, 1986.
[17] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.
[18] X. Li, Y. Li, J. Song, The asymptotic value of graph energy for random graphs with degree-based weights, Discrete Appl. Math. 284 (2020) 481–488.
[19] J.X. Li, J.M. Guo, W.C. Shiu, MATCH Commun. Math. Comput. Chem. 74 (2015) 389–398.
[20] B. Liu, Y. Huang, J. Feng, A note on the Randić spectral radius, MATCH Commun. Math. Comput. Chem. 68 (2012) 913–916.
[21] J. Monsalve, J. Rada, Vertex-degree-based topological indices of digraphs, Discrete Appl. Math. 295 (2021) 13–24.
[22] J. Monsalve, J. Rada, Sharp upper and lower bounds of VDB topological indices of digraphs, Symmetry 13 (2021) 1093.
[23] J. Monsalve, J. Rada, Energy of a digraph with respect to a VDB topological index, Spec. Matrices 10 (2022) 417–426.
[24] V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 320 (2007) 1472–1475.
[25] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.
[26] M. Randić, M. Novič, D. Plavšić, Solved and Unsolved Problems in Structural Chemistry, CRC Press, Boca Raton, 2016.
[27] Y. Shao, Y. Gao, W. Gao, X. Zhao, Degree-based energies of trees, Linear Algebra Appl. 621 (2021) 18–28.
[28] P.M. Weichsel, The Kronecker product of graphs, Proc. Am. Math. Soc. 13 (1963) 47–52.