Energy and Randić index of directed graphs

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ABSTRACT

The concept of Randić index has been extended recently for a digraph. We prove that

\[2R(G) \leq \mathcal{E}(G) \leq 2\sqrt{\Delta(G)} R(G),\]

where \(G\) is a digraph, and \(R(G)\) denotes the Randić index, \(\mathcal{E}(G)\) denotes the Nikiforov energy and \(\Delta(G)\) denotes the maximum degree of \(G\). Moreover, in both inequalities, we describe the graphs for which the equality holds. We also develop the concept of inner and outer energies of a vertex for directed graphs extending important inequalities known for the energy of a vertex for graphs.

ARTICLE HISTORY

Received 14 January 2022
Accepted 18 July 2022

COMMUNICATED BY

J. Y. Shao

KEYWORDS

Randić index; graph energy; digraphs; vertex energy

MSC 2010

05C50; 05C09

1. Introduction

The energy of graph and the Randić index are well-known graph invariants defined from considerations in chemical graph theory. These two quantities are known to be good descriptors of any graph and their properties have been explored in networks. Since for many networks, the relation between nodes is non-symmetric, it is natural to study these descriptors for directed graphs, where, for example, the inner and outer degrees play very different roles in terms of the ‘flow’ structure of the network.

The following inequalities have been proven in Refs. [1,2]:

\[2R(G) \leq \mathcal{E}(G) \leq 2\sqrt{\Delta(G)} R(G),\]  \hspace{1cm} (1)

where \(G\) is an (undirected) simple graph, \(R(G)\) the Randić index of \(G\), \(\mathcal{E}(G)\) the energy of \(G\) and \(\Delta(G)\) the maximum degree of \(G\). A notion of energy of a digraph was defined in Ref. [3]. Recently, the definition of Randić index has been extended and studied for digraphs [4,5].

In this paper, we extend (1) to directed graphs. We give two proofs of these inequalities, each of them giving different insights and using different methods. We believe that these methods can be useful in understanding relations between the energy of a graph and vertex degree-based indices.

The first method involves extending the definition of vertex energy to digraphs. The vertex energy has proven to give new results in the area (see for example [1,2,6–8]). In
the way, we extend known inequalities for the vertex energy of a graph to digraphs. We note that since the adjacency matrix of a directed graph is not necessarily symmetric and our definitions of energy and Randić index change, we need to adapt the previous known methods and proofs. In particular, we define inner and outer energies, which we relate with the inner and outer degrees.

The second method is what we call the Hermitianization trick, which relates concepts such as the energy and vertex degree-based indices of a digraph with the corresponding concepts of a bipartite undirected graph. With further analysis, this allows us to describe the directed graphs for which the equalities in (1) hold. To the best of our knowledge, this trick was first used to study the energy of graphs in Ref. [7], but it is well known in Random Matrix Theory and known as Girko Hermitianization trick [9].

Apart from this introduction, the paper is organized as follows. In Section 2, we introduce the energy of a digraph as defined by Nikiforov. We also define the outer energy of a vertex $E^+(v)$ and inner energy of a vertex $E^-(v)$ and prove that for adjacent vertices $E^+(v_1)E^-(v_2) \geq 1$. In Section 3, we prove the main results of the paper, namely that inequalities in (1) are satisfied for digraphs and their corresponding Randić index and energy. Section 4 is devoted to the Hermitianization trick. We use this technique to give another proof of the main theorems of the paper and to describe the graphs in which the equalities in (1) are fulfilled.

2. Digraph energy and vertex energy

A (finite) directed graph or digraph is a pair $G = (V, E)$ where $V$ is a finite set and $E \subseteq V \times V$, the elements in $V$ are called vertices and the elements in $E$ are called edges. We assume that $G$ is simple, i.e. $(v, v) \notin E$ for all $v \in V$. For a digraph $G$ with $n$ vertices, the adjacency matrix, denoted by $A = A(G)$, is the $n \times n$ matrix with entries $A_{ij} = 1$ if $(v_i, v_j) \in E$ and $A_{ij} = 0$ otherwise.

The energy of a graph is given by the trace of the absolute value of its adjacency matrix [10–12]. In analogy to graphs, the energy of a digraph is defined as follows. Let us consider a digraph $G = (V, E)$ with adjacency matrix $A \in M_n(\mathbb{R})$. One can define the absolute value of $A$ in two ways:

$$|A|^+ = (AA^t)^{1/2},$$
$$|A|^− = (A^tA)^{1/2},$$

where, for a positive matrix $M$, $M^{1/2}$ denotes the unique positive matrix such that $(M^{1/2})^2 = M$. Both definitions coincide when $A$ is symmetric, i.e. $G$ is undirected.

**Definition 2.1 ([13]):** The energy of a digraph $G$, denoted $\mathcal{E}(G)$, is given by

$$\mathcal{E}(G) = \text{Tr}(|A|^+) = \text{Tr}(|A|^−),$$

where $A$ is the adjacency matrix of $G$. 

Note that,
\[ E(G) = \sum_{i=1}^{n} \sigma_i, \]
where \((\sigma_i)_{i=1}^{n}\), denote the set of singular values of \(A(G)\), counted with multiplicities.

In Ref. [7], the energy of a vertex is introduced. We extend this definition to digraphs.

**Definition 2.2:** The outer energy of the vertex \(v_i\) with respect to \(G\), which is denoted by \(E_G^+(v_i)\), is given by
\[ E_G^+(v_i) = |A|^{-1}_{ii}, \quad \text{for } i = 1, \ldots, n, \] (2)
where \(|A|^{-1} = (AA^t)^{1/2}\) and \(A\) is the adjacency matrix of \(G\).

**Definition 2.3:** The inner energy of the vertex \(v_i\) with respect to \(G\), which is denoted by \(E_G^-(v_i)\), is given by
\[ E_G^-(v_i) = |A|^{-1}_{ii}, \quad \text{for } i = 1, \ldots, n, \] (3)
where \(|A|^{-1} = (A^tA)^{1/2}\) and \(A\) is the adjacency matrix of \(G\).

In this way the energy of a graph is given by the sum of the individual energies of the vertices of \(G\),
\[ E(G) = E_G^+(v_1) + \cdots + E_G^+(v_n) = E_G^-(v_1) + \cdots + E_G^-(v_n). \]

It is important to remark, as observed by Ref. [14] that, in general, the inner and outer energy of a vertex do not coincide.

### 2.1. Energy of adjacent vertices

The next theorem is fundamental for the proof of our main result.

**Theorem 2.1:** Let \((v_i, v_j)\) be an arc of a simple digraph \(G\). Then \(E_G^+(v_i)E_G^-(v_j) \geq 1\).

**Proof:** Let \(A(G)\) be the adjacency matrix of \(G\). Then, using the singular decomposition, we can write \(A(G) = U\Sigma V^t\), where \(U = (u_{kl})\), \(V = (v_{kl})\) are orthogonal and \(\Sigma = (\sigma_{kl})\) is a diagonal matrix with non negative entries. Let us denote \(\sigma_{kk} = \sigma_k\). From this, we have that \(AA^t = U\Sigma^2 U^t\) and \(A^tA = V\Sigma^2 V^t\), hence
\[ |A|^{+} = U\Sigma U^t, \]
\[ |A|^{-} = V\Sigma V^t. \]

A direct calculation shows that \(E_G^+(v_i) = \sum_k u_{ik}^2\sigma_k\) and \(E_G^-(v_j) = \sum_k v_{jk}^2\sigma_k\). Moreover \(A(G)_{ij} = \sum_k u_{ik}v_{jk}\sigma_k\). Since \((v_i, v_j)\) is an arc then \(A(G)_{ij} = 1\).
Now consider
\[ u = (u_1 \sqrt{\sigma_1}, \ldots, u_n \sqrt{\sigma_n}) \]
and
\[ v = (v_1 \sqrt{\sigma_1}, \ldots, v_n \sqrt{\sigma_n}) \]
then
\[ \langle v, w \rangle^2 = \left( \sum_k u_{ik} v_{jk} \sigma_k \right)^2 = 1 \]
\[ \|v\|^2 = \sum_k u_{ik}^2 \sigma_k = E^+(v_i) \]
\[ \|w\|^2 = \sum_k v_{jk}^2 \sigma_k = E^-(v_j) \]
which proves the assertion by the Cauchy-Schwarz inequality.

By the use of AM-GM inequality we observe that:

**Corollary 2.1:** Let \((v_i, v_j)\) be an arc of a simple digraph \(G\). Then \(E^+(v_i) + E^-(v_j) \geq 2\).

### 3. Randić index and energy of digraphs

Let \(G = (V, E)\) be a digraph. For a vertex \(v \in V\), we denote by \(d^+(v)\) and \(d^-(v)\), the outer and inner degrees of \(v\), respectively, given by the cardinality of the sets
\[ N^+(v) = \{ w \in V | (v, w) \in E \} \quad \text{and} \quad N^-(v) = \{ w \in V | (v, w) \in E \}. \]

We denote by \(a\) the number of edges (or arcs), i.e. \(a = |E|\). Observe that \(\sum_{v \in V} d^+(v) = a = \sum_{v \in V} d^-(v)\). We denote by \(\Delta(G)\) the maximum, over the vertices, of the inner and outer degrees.

For a digraph \(G = (V, E)\), the Randić index was defined in Ref. [5] and is given by
\[ R(G) = \frac{1}{2} \sum_{(v, w) \in E} \frac{1}{\sqrt{d^+(v)d^-(w)}}. \]

where \(d^+(v)\) and \(d^-(v)\) correspond to the outer and inner degrees of \(v\).

**Theorem 3.1:** Let \(G\) be a digraph with energy \(E(G)\) and Randić index \(R(G)\) then \(E(G) \geq 2R(G)\).

**Proof:** Let \(G = (V, E)\). For an edge \(e = (v, w)\) define \(E(e) = E^+(v)/d^+(v) + E^-(w)/d^-(w)\). Then, on the one hand,
\[ \sum_{e \in E} E(e) = \sum_{e \in E} \left( \frac{E^+(v)}{d^+(v)} + \frac{E^-(w)}{d^-(w)} \right) \]
On the other hand, by the classical AM-GM inequality, if \( e = (v, w) \),

\[
\mathcal{E}(e) := \frac{\mathcal{E}^+(v)}{d^+(v)} + \frac{\mathcal{E}^-(w)}{d^-(w)} \geq 2 \sqrt{\frac{\mathcal{E}^+(v)\mathcal{E}^-(w)}{d^+(v)d^-(w)}} \geq 2 - \frac{1}{\sqrt{d^+(v)d^-(w)}},
\]

where we used Theorem 2.1 in the last inequality.

Finally, summing over \( e \in E(G) \) we obtain the desired inequality

\[
\mathcal{E}(G) = \frac{1}{2} \sum_{e \in E(G)} \mathcal{E}(e) \geq \sum_{(v, w) \in E(G)} \frac{1}{\sqrt{d^+(v)d^-(w)}} = 2R(G)
\]

Now we prove an analogous result to the one in Ref. [6] for digraphs, relating the vertex energy with the degree.

**Lemma 3.1:** For a digraph \( G \) and a vertex \( v_i \in G \)

\[
\mathcal{E}^+(G)(v_i) \leq \sqrt{d^+(i)},
\]

and

\[
\mathcal{E}^-(G)(v_i) \leq \sqrt{d^-(i)}.
\]

**Proof:** We only prove the first inequality, the other one is analogous and also follows by taking \( \tilde{G} \), which is the graph with the same edges as \( G \) but with the directions reversed, i.e. \( (v, w) \in G \) if and only if \( (w, v) \in \tilde{G} \).

Let \( A(G) \) be the adjacency matrix of \( G \). Then, using the singular decomposition, we can write \( A(G) = UDV^t \), where \( U = (u_{ki}) \) and \( V = (v_{ki}) \) are orthogonal matrices and \( D = (d_{ki}) \) is diagonal. Let us denote \( d_{kk} = \sigma_k \). From this, we have that \( AA^t = UD^2U^t \) and \( |A|^t = U|D||U^t \). Again, \( \mathcal{E}^+(v_i) = \sum_k u_{ik}^2|\sigma_k| \). Observe now that the elements of the diagonal in \( AA^t \) give us the outer degrees of \( G \) hence \( d^+(i) = (AA^t)_{ii} = \sum_k u_{ik}^2\sigma_k^2 \).

Now consider the vectors \( v = (u_{i1}|\sigma_1|, \ldots, u_{in}|\sigma_n|) \) and \( w = (u_{i1}, \ldots, u_{in}) \) then we have that

\[
\mathcal{E}^+(v_i)^2 = \left( \sum_k u_{ik}^2|\sigma_k| \right)^2 \leq \sum_k u_{ik}^2\sigma_k^2 \sum_k u_{ik}^2 = \sum_k u_{ik}^2\sigma_k^2 = d^+(v_i)
\]

where the inequality follows by the Cauchy-Schwarz inequality for \( v \) and \( w \).

As a corollary, we obtain a McClelland’s type inequality for the graph.
**Corollary 3.1:** For a simple digraph $G$ with $n$ vertices and $a$ edges. Then

$$\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i^+} \leq \sqrt{an},$$

and

$$\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i^-} \leq \sqrt{an}.$$

**Proof:** The first (third) inequality follows by summing the outer (inner) energies and comparing each one with the respective outer (inner) degrees. The second (last) one follows using QM-AM inequality since $\sum d_i^+ = a \left( \sum d_i^- = a \right)$.

**Theorem 3.2:** Let $G$ be a digraph with energy $\mathcal{E}(G)$, Randić index $R(G)$ and maximum degree $\Delta(G)$ then $\mathcal{E}(G) \leq 2\sqrt{\Delta(G)}R(G)$.

**Proof:**

$$\mathcal{E}(G) = \frac{1}{2} \sum_{e \in \mathcal{E}(G)} E(e)$$

$$= \frac{1}{2} \sum_{(v,w) \in \mathcal{E}(G)} \frac{\mathcal{E}^+(v)}{d^+(v)} + \frac{\mathcal{E}^-(w)}{d^-(w)}$$

$$\leq \frac{1}{2} \sum_{(v,w) \in \mathcal{E}(G)} \frac{\sqrt{d^+(v)}}{d^+(v)} + \frac{\sqrt{d^-(w)}}{d^-(w)}$$

$$= \frac{1}{2} \sum_{(v,w) \in \mathcal{E}(G)} \frac{1}{\sqrt{d^+(v)}} + \frac{1}{\sqrt{d^-(w)}}$$

$$= \frac{1}{2} \sum_{(v,w) \in \mathcal{E}(G)} \frac{\sqrt{d^+(v)} + \sqrt{d^-(v)}}{\sqrt{d^+(v)}d^-(w)}$$

$$\leq (2\sqrt{\Delta(G)}) \left( \frac{1}{2} \sum_{(v,w) \in \mathcal{E}(G)} \frac{1}{\sqrt{d^+(v)}d^-(w)} \right)$$

$$= (2\sqrt{\Delta(G)})R(G) \quad \blacksquare$$

4. **Hermitianization trick**

In this section, we give alternative proofs of Theorems 3.1 and 3.2. We use the construction relating different energies first observed in Ref. [7]. We notice that, independently, Monsalve and Rada [15], made an equivalent construction (modulo some isolated vertices).

However, we believe that the construction used here gives a clearer and more direct way of relating directed graphs with bipartite ones since we directly use the adjacency matrix to define it, while the construction in [15] uses a splitting/replacement scheme.
4.1. Nikiforov’s energy and \((n, m)\)-bipartite graphs

Recall [3], that for a matrix \(M\) the (Nikiforov) energy of \(M, N(M)\), is given by

\[
\text{Tr}(\sqrt{MM^T}) = \sum_{i}^{n} \sigma_i(M),
\]

where \((\sigma_i(M))_{i=1}^{n}\) denotes the set of singular values of \(M\).

Now, the adjacency matrix \(A\) of a bipartite graph whose parts have \(r\) and \(s\) vertices has the form

\[
A = \begin{pmatrix}
0_{r \times r} & M \\
M^T & 0_{s \times s}
\end{pmatrix}, \quad (4)
\]

where \(M\) is a \((0, 1)\)-matrix of size \(r \times s\), and \(0\) represents the zero matrix. Conversely, given a \((0, 1)\)-matrix \(M\) of size \(r \times s\), the matrix \(A\) as in (4) is the adjacency matrix of a bipartite graph. Thus there is a one-to-one correspondence between \((r, s)\)-bipartite graphs and \((0, 1)\)-matrices of size \(r \times s\).

Moreover, it easily follows from the singular value decomposition that for any matrix \(M\), the non-zero eigenvalues of the matrix \(A\) in (4) are the nonzero singular values of \(M\) together with their negatives and thus for any bipartite graph \(G\) with adjacency matrix \(A\) as in (4), one has

\[
E(G) = 2N(M). \quad (5)
\]

In other words, studying the energy of \((r, s)\)-bipartite graphs corresponds to studying Nikiforov’s energy of \((0, 1)\)-matrices of size \(r \times s\).

4.2. Digraphs and \((n, n)\)-bipartite graphs

We are interested in the particular case when \(r = s = n\).

Let \(G = (V, E)\) be a directed graph on \(V = \{1, \ldots, n\}\). We denote by \(B(G) = (\overline{V}, \overline{E})\) the undirected bipartite graph with vertex set \(\overline{V} = \{1^-, \ldots, n^-, 1^+, \ldots, n^+\}\) and edge set described as follows: \((i, j) \in E\) if and only if \([i^-, j^+] \in \overline{E}\), i.e \(i \to j \iff i^- \sim j^+\).

Moreover, the relation between the adjacency matrices of these graphs is as in (4). Thus, from (5), we obtain a direct relation between their energies (Figure 1).
**Corollary 4.1:** For any directed graph $G$,

$$2\mathcal{E}(G) = \mathcal{E}(B(G)).$$  \hspace{1cm} (6)

In order to prove our main theorem, we need to relate the Randić index of $G$ with the Randić index of $B(G)$, which amounts relating their degrees.

**Lemma 4.1:** For any directed graph $G$ with vertex set $[n] = \{1, \ldots, n\}$, and $B(G)$ with vertex set $\{1^-, \ldots, n^-, 1^+, \ldots, n^+\}$, the following relations holds, for any $i \in [n]$:  

$$d^+(i) = d(i^+), \quad d^-(i) = d(i^-),$$

where $d^+ : V \to \mathbb{N}$, $d^- = V \to \mathbb{N}$ denote the out-degree and in-degree in $G$, and $d : V \to \mathbb{N}$ denotes degree in $B(G)$.

**Proof:** This is clear by taking cardinalities in set relations  

$$|\{j \in [n] | i \to j\}| = |\{j \in [n] | i^-\to j^+\}|$$

and  

$$|\{i \in [n] | i \to j\}| = |\{i \in [n] | i^- \to j^+\}|.$$  \hspace{1cm} ■

From the above simple lemma one then sees that $2R(G) = R(B(G))$.

**Corollary 4.2:** For any directed graph $G$

$$2R(G) = R(B(G)).$$  \hspace{1cm} (7)

**Proof:** Since $(i, j) \in E(G)$ exactly when $\{i^-, j^+\} \in E(B(G))$, and any edge in $E(B(G))$ is of the form $\{i^-, j^+\}$, for some $i, j \in [n]$, then

$$2R(G) = \sum_{(i,j) \in E(G)} \frac{1}{\sqrt{d^+(i)d^-(j)}},$$  \hspace{1cm} (8)

$$= \sum_{\{i^-, j^+\} \in E(B(G))} \frac{1}{\sqrt{d(i^+)d(j^-)}},$$  \hspace{1cm} (9)

$$= R(B(G)).$$  \hspace{1cm} (10)  \hspace{1cm} ■

**Remark 4.1:** The obvious generalization to any vertex-degree-based topological index holds. In particular, for the generalized Randić index.

**Remark 4.2:** Corollary 4.1, may be compared with in [15, Theorem 2.5]. Similarly, Lemma 4.1 should be compared with [16, Proposition 2.4].

Now we are ready to prove Theorems 3.1 and 3.2.
Figure 2. Decomposition of a graph into sink-source graphs.

**Proof:** These follow from Corollaries 4.1 and 4.2, together with Equation (1), applied to $B(G)$. Indeed,

$$2R(G) = R(B(G)) \leq \frac{1}{2}E(B(G)) = E(G) \quad (11)$$

and

$$E(G) = \frac{1}{2}E(B(G)) \leq \sqrt{\Delta(B(G))}R(B(G)) = 2\sqrt{\Delta(G)}R(G) \quad (12)$$

\[\blacksquare\]

**4.3. Graphs attaining equalities**

Given a digraph $G = (V, G)$, a vertex $v \in G$ is called a sink vertex if $d^+(v) = 0$ and is called a source vertex if $d^-(v) = 0$. We say that $G$ is a sink-source digraph if every vertex of $G$ is either a sink or a source.

A sink-source digraph can be thought as a bipartite graph since we can split the set of vertices $V$ into two subsets $V_1, V_2$ and such that $ij \in E$ if and only if $i \in V_1$ and $j \in V_2$, moreover if $G$ there is a 2-to-1 correspondence between weakly connected sink-source digraphs and connected bipartite graphs given by choosing the sink and the source sets (see [15, Proposition 2.2]).

**Definition 4.1:** A splitting of a digraph $G$ into sink-source digraphs is a set $\{G_1, \ldots, G_n\}$ of sink-source digraphs such that $G = \bigcup_{i=1}^n G_i$ with the condition that $d^+_{G_i}(v) \neq 0$ implies $d^+_{G}(v) = d^+_{G_i}(v)$.

**Example 4.1:** Consider the graph $G$ with vertex set $V = \{1, 2, 3, 4, 5\}$ and edge set $E = \{(1, 4), (1, 5), (2, 4), (5, 1), (5, 2), (5, 3)\}$ then $G$ can be split into sink-source graphs $G_1 = (V_1, E_1) = ((1, 2, 4, 5), \{(1, 4), (1, 5), (2, 4)\})$ and $G_2 = (V_2, E_2) = ((1, 2, 3, 5), \{(5, 1), (5, 2), (5, 3)\})$, see Figure 2.

**Remark 4.3:** Not every digraph admits a splitting into sink-source digraphs. The graph with $V = \{1, 2, 3\}$ and $E = \{(1, 2), (1, 3), (2, 3)\}$ doesn’t admit a splitting into sink-source digraphs.
Theorem 4.1: Let $G$ be a digraph, then $\mathcal{E}(G) = 2R(G)$ if and only if there is a splitting of $G$ into sink-source digraphs $\{G_1, \ldots, G_k\}$ such that $G_i = \overrightarrow{K}_{n_i,m_i}$, for some $n_i, m_i \in \mathbb{N}$.

Proof: Given a digraph $G$, by using the Hermitianization trick then $\mathcal{E}(G) = 2R(G)$ if and only if $\mathcal{E}(B(G)) = 2R(B(G))$. Suppose then that the equality is satisfied, then by Theorem 6 in Ref. [1], this implies that $B(G)$ is the disjoint union of complete bipartite graphs. Each complete bipartite graph $K_{n_i,m_i} \subset B(G)$ corresponds to a graph $\overrightarrow{K}_{n_i,m_i} \subset G$. For each source vertex $v \in \overrightarrow{K}_{n_i,m_i}$, the fact that the $K_{n_i,m_i}$’s are disjoint implies that $d_+^G(v) = d_B(G)(v^+) = n_i$, analogously, for each sink vertex $v \in \overrightarrow{K}_{n_i,m_i}$ we have that $d_-^G(v) = d_B(G)(v^-) = m_i$. Hence $\{\overrightarrow{K}_{n_1,m_1}, \ldots, \overrightarrow{K}_{n_k,m_k}\}$ is a splitting into sink-source digraphs.

Conversely, suppose that there is a splitting of $G$ into sink-source digraphs, $\{\overrightarrow{K}_{n_1,m_1}, \ldots, \overrightarrow{K}_{n_k,m_k}\}$. Now, let $v \in \overrightarrow{K}_{n_i,m_i}$ be a source, then $n_i = d_+^G(v)$, by the degree conditions of a splitting into sink-source digraphs. Similarly, for each sink $w \in \overrightarrow{K}_{n_i,m_i}$ we have that $m_i = d_-^G(w)$.

Now, let $V_i = \{v_1^i, \ldots, v_{n_i}^i\}$ denote the set of sources of $\overrightarrow{K}_{n_i,m_i}$ and $W_i = \{w_1^i, \ldots, w_{m_i}^i\}$ the set of sinks. Since $n_i = d_+^G(v)$ then $(v_k^i, w_j^i) \in E(G)$ implies that $w = w_k^i$ for some $k \in \{1, \ldots, m_i\}$, analogously, since $m_i = d_-^G(w)$, then $(v, w_j^i) \in E(G)$ implies that $v = v_k^i$ for some $k \in \{1, \ldots, n_i\}$, that is, the edges that start in $V_i$ always end in $W_i$ and the edges that end in $W_i$ always start in $V_i$. The corresponding graph in $B(G)$ is a complete bipartite graph $K_{n_i,m_i}$ with the set $V_i^+ = \{(v_1^i)^+ \ldots, (v_{n_i}^i)^+\}$ connected to the set $W_i^- = \{(w_1^-)^i \ldots, (w_{m_i}^-)^i\}$ which is disjoint with other graphs since, the last statement implies that all the elements of $V_i^+$ are only connected with the elements of $W_i^-$ and all the elements of $W_i^-$ are only connected with the elements of $V_i^+$. Consequently, $B(G)$ is a union of complete bipartite graphs and $\mathcal{E}(B(G)) = 2R(B(G))$. This completes the proof.

Lemma 4.2: Let $G$ be a weakly connected finite simple digraph such that for all vertices $d^+(v) \leq 1$ then $G$ is either a directed path or a directed cycle.

Proof: Let $n$ be the number of elements in $G$. If $n = 1$ then $G$ is an isolated vertex.

When $n > 1$ we divide into two cases.

Case 1. There is a vertex $v_1$ with $d^+(v_1) = 0$. Then $d^+(v) = 1$ which means that there is a unique element $v_2$ such that $(v_1, v_2)$ is an edge, if $n > 2$ then $d^+(v) = 1$ since, if this is false, we will have that $\{v_1, v_2\}$ is a weakly connected component of $G$ because there cannot be other edges pointing $v_2$ by the fact that $d^-(v_2) \leq 1$. So there is a unique element $v_3$ such that $(v_2, v_3)$ is an edge. Inductively, there should be a sequence of vertices $v_1, \ldots, v_n$ such that $(v_i, v_{i+1}) \in E(G)$ for all $i \in \{1, \ldots, n - 1\}$. This means $G$ is a directed path.

Case 2. There is a vertex $v_1$ with $d^-(v_1) = 0$. The same proof as case 1 works with obvious modifications.

Case 3. For every vertex $v \in V$, $d^+(v) = d^-(v) = 1$. Take now any vertex $v_1 \in V$ then since for every vertex $d^+(v) = 1$ we can form unique sequence of vertices $\{vi\}_{i \in \mathbb{N}}$ such that $(v_i, v_{i+1}) \in E(G)$ since the graph is finite, this sequence should repeat. That is, there is some $k$ and $l$ such that $v_{k+l} = v_l$. Now, consider the directed path $v_i \rightarrow v_{i+1} \rightarrow v_{i+k} = v_l$. For each $v_i$, since $d^+(v) = d^-(v) = 1$, there is a unique $w$ such that $w, v_i \in E(G)$, which should be $v_{i-1}$ and similarly, $v_{i+1}$ is the unique vertex after $v_i$. This means that $\{v_l, \ldots, v_{k+l}\}$ is
directed cycle and a weakly connected component. Thus \( k = n \) and \( G \) must be this directed cycle.

\[ \text{Theorem 4.2: Let } G \text{ be a digraph with energy } E(G) \text{ and Randić index } R(G) \text{ and maximum degree } \Delta(G) \text{ then } E(G) = 2\sqrt{\Delta(G)}R(G) \text{ if and only if } G \text{ is the disjoint union of directed cycles } \overrightarrow{C_n}, \text{ directed paths } \overrightarrow{P_n} \text{ and isolated vertices.} \]

\[ \text{Proof: Suppose that } G \text{ is a disjoint union of directed paths or directed cycles then since for each edge } (i, j) \text{ it holds that } d^+_i = d^-_j = 1 \text{ then } R(G) = 1/2a \text{ where } a \text{ is the number of arcs. A direct calculation shows that } E(\overrightarrow{C_n}) = n \text{ and } E(\overrightarrow{P_n}) = n - 1, \text{ which coincides with their number of arcs.} \]

Now suppose that the equality holds. Since \( \Delta(G) = \Delta(B(G)) \) and \( 2R(G) = R(B(G)) \) and \( 2E(G) = E(B(G)) \) then the equality holds if and only if it holds for \( B(G) \). Using Theorem 16 in Ref. [2], this is equivalent to \( B(G) \) being the disjoint union of the path \( P_2 \) and isolated vertices. Since all degrees in \( B(G) \) are either 0 or 1 this implies that all in-degrees and out-degrees of \( G \) are also 0 or 1. The use of Lemma 4.2 finishes the proof.

\[ \text{Acknowledgments} \]

The author thanks Roland Speicher and Moritz Weber for the nice environment at University of Saarlands, while visiting for a sabbatical period.

\[ \text{Disclosure statement} \]

No potential conflict of interest was reported by the authors.

\[ \text{Funding} \]

O.A. received support from Conacyt (Consejo Nacional de Ciencia y Tecnología) [grant number CB-2017-2018-A1-S-9764] and from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no 734922.

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