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Original Scientific Paper

On Reciprocal and Reverse Balaban Indices*

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Abstract. The Ivanciuc-Balaban operator of a graph G is defined as

$$J(\mathbf{M},G)=\frac{m}{\mu+1}\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}$$

where **M** is its molecular matrix with positive row-sums, m is the number of edges, μ is the cyclomatic number, M_i is the i-th row sum of **M** and the summation goes over all edges from the edge-set $E(G)$. Here we consider the reciprocal Balaban index $^{r}J(G)=J(\mathbf{RD},G)$ and the reverse Balaban index $J_r(G)=J(\mathbf{RW},G)$, where **RD** and **RW** are respectively the reciprocal distance matrix and the reverse Wiener matrix of G. Various lower and upper bounds for these two types of Balaban-like indices are reported.

Keywords: Ivanciuc-Balaban operator, Balaban index, reciprocal Balaban index, reverse Balaban index

INTRODUCTION

The distance matrix and related matrices, based on graph-theoretical distances,[1] are rich sources of many graph invariants (molecular descriptors, topological indices) that found use in the structure-property-activity modeling.[2–4] We consider simple connected (molecular) graphs.[5] Let G be a connected graph with vertex-set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge-set $E(G)$.

For a symmetric $n\times n$ molecular matrix $\mathbf{M}=\mathbf{M}(G)$ whose (i,j)-entry is $\mathbf{M}_{ij}$, where $i,j = 1, 2,\ldots,n$, let $M_i=\sum_{i=1}^{n}\mathbf{M}_{ij}$ be the sum of the entries in row i of **M**. Suppose that $M_i>0$ for $i=1,2,\ldots,n$. The Ivanciuc-Balaban operator of the graph G and **M** is defined as[6]

$$J(\mathbf{M},G)=\frac{m}{\mu+1}\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}$$

where m is the number of edges and μ is the cyclomatic number or the circuit rank[7] of G. Note that $\mu = m - n + 1$. We point out that $\mathbf{IB}(\mathbf{M},G)$ is used instead of $J(\mathbf{M},G)$ in Ref. 6.

The distance matrix **D** of the graph G is an $n\times n$ matrix $(\mathbf{D}_{ij})$ such that $\mathbf{D}_{ij}$ is just the distance (*i.e.*, the number of edges of a shortest path) between the vertices v_i and v_j in G.[1] The reciprocal distance matrix **RD** of G is an $n\times n$ matrix $(\mathbf{RD}_{ij})$ such that[1,8,9]

$$\mathbf{RD}_{ij}=\begin{cases}\dfrac{1}{\mathbf{D}_{ij}} & \text{if } i\neq j\\[2mm] 0 & \text{if } i=j\end{cases}$$

Let d be the diameter (maximum possible distance between any two vertices)[7] of the graph G. The reverse Wiener matrix **RW** of G is an $n\times n$ matrix such that[10]

$$\mathbf{RW}_{ij}=\begin{cases}d-\mathbf{D}_{ij} & \text{if } i\neq j\\ 0 & \text{if } i=j\end{cases}$$

It is easily seen that $J(\mathbf{D},G)$ is the Balaban index (also called the average distance sum connectivity) of the (non-weighted) graph G,[11,12] which has been used successfully in developing QSAR/QSPR models[4] and in drug design, *e.g.*, Ref. 13. Recently, we presented in this journal some properties of the Balaban index.[14] Thus, this report represents a natural extension of the previous

* Dedicated to Professor Emeritus Drago Grdenić, Fellow of the Croatian Academy of Sciences and Arts, on the occasion of his 90th birthday.
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study to properties of related Balaban-type molecular descriptors.

Molecular descriptor denoted by $J(\mathbf{RD},G)$ is called the reciprocal Balaban index (also called the Harary-Balaban index[15] and the Harary-connectivity index[16]) of the graph G, denoted by ${}^rJ$ or ${}^rJ(G)$. We call $J(\mathbf{RW},G)$ the reverse Balaban index of the graph G, denoted by J_r or $J_r(G)$. Note that J_r makes sense only for non-complete connected graphs. It has also been shown that the reciprocal and reverse Balaban indices are able to produce fair QSPR models for molar heat capacity, standard Gibbs energy of formation, refractive index and vaporization enthalpy for C_6 - C_{10} alkanes.[17] Other applications of the Ivanciuc-Balaban operator were presented in Ref. 18.

In this report, we present some properties of the reciprocal and reverse Balaban indices, especially their lower and upper bounds.

PRELIMINARIES

The Wiener operator of a graph G with n vertices, whose molecular matrix $\mathbf{M}$ is symmetric with zero diagonal, is defined as

$$\mathrm{Wi}(\mathbf{M},G) = \sum_{i<j} \mathbf{M}_{ij} = \frac{1}{2}\sum_{i=1}^{n} M_i$$

Note that $W(G) = \mathrm{Wi}(\mathbf{D},G)$ is the Wiener index as defined by Hosoya,[19] $H(G) = \mathrm{Wi}(\mathbf{RD},G)$ is the Harary index,[8,9,20–23] and

$$\Lambda(G) = \mathrm{Wi}(\mathbf{RW},G) = \frac{1}{2}n(n-1)d - W(G)$$

is the reverse Wiener index[10,24] of G.

For a graph G and $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $\delta_i = |\Gamma(v_i)|$. The adjacency matrix $\mathbf{A}$ of G is an $n \times n$ matrix $(\mathbf{A}_{ij})$ such that $\mathbf{A}_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise.[1] Since $\mathbf{A}$ is symmetric, its eigenvalues are real. Let $\rho = \rho(G)$ be the maximum eigenvalue (of the adjacency matrix) of G, which has been proposed by Cvetković and Gutman[25] as the measure of molecular branching. For more details on the properties of ρ, see the monograph on spectra of graphs by Cvetković *et al.*[26]

A graph is a semiregular bipartite graph of degrees r_1, r_2 if it is bipartite and each vertex in one part of the bipartition has degree r_1 and each vertex in the other part of the bipartition has degree r_2.[7] Let K_n be the complete graph with n vertices.[7] The superscript T denotes the transpose of a vector.

Lemma 1.[27,28] Let G be a connected graph on n vertices with adjacency matrix $\mathbf{A}$. Let $\mathbf{x}$ be an n-dimensional column vector with positive entries. Then $\rho \ge \dfrac{\mathbf{x}^T\mathbf{A}\,\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$ with equality if and only if $\mathbf{x}$ is an eigenvector belonging to ρ.

Lemma 2.[29] Let G be a connected graph with n vertices and m edges. Then $\rho \le \sqrt{2m-n+1}$ with equality if and only if G is the star or the complete graph.

RESULTS

The following proposition applies to the Balaban index ($\mathbf{M} = \mathbf{D}$),[11] the reciprocal Balaban index ($\mathbf{M} = \mathbf{RD}$) for connected graphs, and the reverse Balaban index ($\mathbf{M} = \mathbf{RW}$) for non-complete connected graphs.

Proposition 3. Let G be a connected graph on n vertices and let $\mathbf{M}$ be a symmetric molecular matrix of G with positive row sums, where the entries of $\mathbf{M}$ on the main diagonal are zero. Then

$$\begin{aligned}\frac{m^3}{(m-n+2)\rho\,\mathrm{Wi}(\mathbf{M},G)} &\le J(\mathbf{M},G) \le \\ &\frac{m\rho}{2(m-n+2)}\sum_{v_i\in V(G)}\frac{1}{M_i}\end{aligned} \tag{1}$$

with left equality if and only if G is either a regular graph such that M_i is a constant for every $v_i \in V(G)$ or a semiregular bipartite graph of degrees, say r_1, r_2 such that $r_1/r_2 = M_i/M_j$ for any vertex v_i in the part with degree r_1 and any vertex v_j in the other part with degree r_2, and with right equality if and only if $\sum_{v_j\in\Gamma(v_i)} M_j^{-1/2} = \rho M_i^{-1/2}$ for any $v_i \in V(G)$.

Proof. Setting $\mathbf{x} = (\sqrt{M_1}, \sqrt{M_2}, \ldots, \sqrt{M_n})^T$ in Lemma 1, we have

$$\rho \ge \frac{1}{\mathrm{Wi}(\mathbf{M},G)}\sum_{v_iv_j\in E(G)}(M_i \cdot M_j)^{1/2}$$

with equality if and only if $\sum_{v_j\in\Gamma(v_i)}\sqrt{M_j} = \rho\sqrt{M_i}$ for any $v_i \in V(G)$. By the Cauchy-Schwarz inequality,

$$\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{1/2} \ge \left[\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/4}(M_i\cdot M_j)^{1/4}\right]^2 = m^2$$

and then

$$\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}\geq\frac{m^2}{\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{1/2}}\geq\frac{m^2}{\rho \mathrm{Wi}(\mathbf{M},G)}$$

from which the left inequality in (1) follows and equality holds if and only if $M_i \cdot M_j$ is a constant for any $v_iv_j \in E(G)$ and $\sum_{v_j\in\Gamma(v_i)}\sqrt{M_j}=\rho\sqrt{M_i}$ for any $v_i \in V(G)$. Note that if $M_i \cdot M_j$ is a constant for any $v_iv_j \in E(G)$ and $\sum_{v_j\in\Gamma(v_i)}\sqrt{M_j}=\rho\sqrt{M_i}$ for any $v_i \in V(G)$, then $\rho\sqrt{M_i}=\delta_i\sqrt{M_j}$ and thus $\delta_i\delta_j=\rho^2$, $\delta_i M_j=\delta_j M_i$ for any $v_iv_j \in E(G)$. Now it is easily seen that equality holds in the left inequality in (1) if and only if G is either a regular graph such that M_i is a constant for every $v_i \in V(G)$ or a semiregular bipartite graph of degrees, say r_1, r_2 such that $r_1/r_2 = M_i/M_j$ for any vertex v_i in the part with degree r_1 and any vertex v_j in the other part with degree r_2.

On the other hand, setting $\mathbf{x}=(M_1^{-1/2},M_2^{-1/2},\ldots,M_n^{-1/2})^T$ in Lemma 1, we have

$$\rho\geq\frac{2\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}}{\sum_{v_i\in V(G)}\frac{1}{M_i}}$$

from which the right inequality in (1) holds and equality holds if and only if $\sum_{v_j\in\Gamma(v_i)}M_j^{-1/2}=\rho M_i^{-1/2}$ for any $v_i \in V(G)$.

If the maximum eigenvalue of the graph G in (1) is replaced by an upper bound, we will have bounds for $J(\mathbf{M},G)$ where ρ does not appear. As an example, by Proposition 3 and Lemma 2, we have:

Proposition 4. Let G be a connected graph with $n \geq 2$ vertices and m edges. Then

$$\frac{m^3}{(m-n+2)\sqrt{2m-n+1}\;H(G)}\leq {}^rJ\leq\frac{m\sqrt{2m-n+1}}{2(m-n+2)}\sum_{v_i\in V(G)}\frac{1}{RD_i}$$

with either equality if and only if $G = K_n$. Moreover, if $n \geq 3$ and $G \neq K_n$, then

$$\frac{m^3}{(m-n+2)\sqrt{2m-n+1}\;\Lambda(G)}\leq J_r<\frac{m\sqrt{2m-n+1}}{2(m-n+2)}\sum_{v_i\in V(G)}\frac{1}{RW_i}$$

with left equality if and only if G is the star.

Let G be a connected graph with $n \geq 2$ vertices and m edges. Note that $H(G)\leq\frac{n(n-1)}{2}$ with equality if and only if $G = K_n$. Thus by the lower bound on ${}^rJ$ in Proposition 4, we have

$${}^rJ\geq\frac{2m^3}{n(n-1)(m-n+2)\sqrt{2m-n+1}}$$

with equality if and only if $G = K_n$.

Proposition 5. Let G be a connected graph with $n \geq 2$ vertices, m edges, maximum degree Δ, minimum degree δ and diameter d. Then

$${}^rJ\leq\frac{m}{2(m-n+2)}\min\left\{\frac{nd\Delta}{n-1+(d-1)\Delta},\frac{2md}{n-1+(d-1)\delta}\right\}\qquad(2)$$

with equality if and only if G is a regular graph and $d \leq 2$.

Proof. It is easily seen that

$$2\sum_{v_iv_j\in E(G)}(RD_i\cdot RD_j)^{-1/2}=\sum_{v_i\in V(G)}\frac{\delta_i}{RD_i}-\sum_{v_iv_j\in E(G)}\left(\frac{1}{\sqrt{RD_i}}-\frac{1}{\sqrt{RD_j}}\right)^2\leq\sum_{v_i\in V(G)}\frac{\delta_i}{RD_i}$$

with equality if and only if $RD_i = RD_j$ for any $v_iv_j \in E(G)$. Since for any $v_i \in V(G)$, $RD_i\geq\frac{n-1+(d-1)\delta_i}{d}$ with equality if and only if the distance between v_i and any other vertex is at most two, and $f(x)=\frac{dx}{n-1+(d-1)x}$ is increasing for $x > 0$, we have

$$\sum_{v_i\in V(G)}\frac{\delta_i}{RD_i}\leq\sum_{v_i\in V(G)}\frac{d\delta_i}{n-1+(d-1)\delta_i}\leq\frac{nd\Delta}{n-1+(d-1)\Delta}$$

with equalities if and only if G is a regular graph of diameter at most two. It is also easily seen that

$$\sum_{v_i\in V(G)}\frac{\delta_i}{RD_i}\leq\sum_{v_i\in V(G)}\frac{d\delta_i}{n-1+(d-1)\delta}\leq\frac{2md}{n-1+(d-1)\delta}$$

with equalities if and only if G is a regular graph of diameter at most two. Now (2) follows easily. From the arguments above, equality holds in (2) if and only if G is a regular graph of diameter at most two and $RD_i = RD_j$ for any $v_iv_j \in E(G)$. Note that if G is a regular graph of diameter at most two, then $RD_i = RD_j$ for any $v_iv_j \in E(G)$. Thus the result follows.

Let $\overline{RD} = \max\limits_{v_i \in V(G)} RD_i$ and $\underline{RD} = \min\limits_{v_i \in V(G)} RD_i$ in Proposition 5. By the Cauchy-Schwarz inequality,

$$\sum_{v_iv_j \in E(G)} \left(\frac{1}{\sqrt{RD_i}} - \frac{1}{\sqrt{RD_j}} \right)^2 \geq$$

$$\frac{1}{m} \left(\sum_{v_iv_j \in E(G)} \left| \frac{1}{\sqrt{RD_i}} - \frac{1}{\sqrt{RD_j}} \right| \right)^2 \geq$$

$$\frac{1}{m} \left(\frac{1}{\sqrt{\underline{RD}}} - \frac{1}{\sqrt{\overline{RD}}} \right)^2 = \frac{(\sqrt{\overline{RD}} - \sqrt{\underline{RD}})^2}{m\overline{RD}\,\underline{RD}}$$

with equalities if and only if $RD_i = RD_j$ for any $v_iv_j \in E(G)$. Then

$$^rJ \leq \frac{m}{2(m-n+2)} \left[\min\left\{ \frac{nd\Delta}{n-1+(d-1)\Delta}, \frac{2md}{n-1+(d-1)\delta} \right\} - \frac{(\sqrt{\overline{RD}} - \sqrt{\underline{RD}})^2}{m\overline{RD}\,\underline{RD}} \right]$$

with equality if and only if G is a regular graph and $d \leq 2$.

Let G be a connected graph with $n \geq 2$ vertices and m edges. By Proposition 5,

$$^rJ \leq \frac{nmd\Delta}{2(m-n+2)[n-1+(d-1)\Delta]} \leq \frac{nm}{2(m-n+2)},$$

$^rJ = \dfrac{nm}{2(m-n+2)}$ if and only if $G = K_n$, and then $^rJ < \dfrac{n(n-1)}{2}$ for $n > 2$.

Proposition 6. Let G be a connected graph with $n \geq 3$ vertices, m edges and diameter $d \geq 2$. Then

$$J_r \leq \frac{nm}{2(m-n+2)(d-1)} \tag{3}$$

with equality if and only if G is a regular graph and $d = 2$.

Proof. It is easily seen that

$$2 \sum_{v_iv_j \in E(G)} (RW_i \cdot RW_j)^{-1/2} =$$

$$\sum_{v_i \in V(G)} \frac{\delta_i}{RW_i} - \sum_{v_iv_j \in E(G)} \left(\frac{1}{\sqrt{RW_i}} - \frac{1}{\sqrt{RW_j}} \right)^2 \leq \sum_{v_i \in V(G)} \frac{\delta_i}{RW_i}$$

with equalty if and only if $RW_i = RW_j$ for any $v_iv_j \in E(G)$. Since for any $v_i \in V(G)$, $RW_i = d(n-1) - D_i \geq d(n-1) - \delta_i - d(n-1-\delta_i) = (d-1)\delta_i$ with equality if and only if the distance between v_i and any other vertex is at most two, we have

$$\sum_{v_i \in V(G)} \frac{\delta_i}{RW_i} \leq \sum_{v_i \in V(G)} \frac{\delta_i}{(d-1)\delta_i} = \frac{n}{d-1}$$

with equality if and only if $d = 2$. Now (3) follows. From the arguments above, equality holds in (3) if and only if $d = 2$ and $RW_i = RW_j$ for any $v_iv_j \in E(G)$, or equivalently, G is a regular graph with $d = 2$.

Let $\overline{RW} = \max\limits_{v_i \in V(G)} RW_i$ and $\underline{RW} = \min\limits_{v_i \in V(G)} RW_i$ in Proposition 6. Then by similar argumentation following the proof of Proposition 5,

$$J_r \leq \frac{m}{2(m-n+2)} \left[\frac{n}{d-1} - \frac{(\sqrt{\overline{RW}} - \sqrt{\underline{RW}})^2}{m\overline{RW}\,\underline{RW}} \right]$$

with equality if and only if G is a regular graph and $d = 2$.

Let G be a connected graph with $n \geq 3$ vertices, m edges, and $G \neq K_n$. By Proposition 6, $J_r \leq \dfrac{nm}{2(m-n+2)}$ with equality if and only if G is a regular graph of diameter two.

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SAŽETAK

O recipročnima i obrnutim Balabanovim indeksima

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Ivanciuc-Balabanov operator grafa G definiran je sljedećim izrazom

$$J(\mathbf{M},G)=\frac{m}{\mu+1}\sum_{v_iv_j\in E(G)}(M_i\cdot M_j)^{-1/2}$$

gdje je **M** molekularna matrica, m broj bridova u grafu G, μ ciklomatski broj, M_i zbroj elementa u i-tom retku molekularne matrice, a zbroj u gornjem izrazu ide preko svih bridova u skupu $E(G)$. Ovdje su razmatrani recipročni Balabanov indeks ${}^{r}J(G)=J(\mathbf{RD},G)$ i obrnuti Balabanov indeks $J_r(G)=J(\mathbf{RW},G)$, gdje je **RD** recipročna matrica udaljenosti, a **RW** obrnuti Wienerov indeks grafa G. Članak sadrži razmatranje o donjim i o gornjim granicama ovih dvaju molekularnih descriptora.