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Original Scientific Article

Bond Additive Modeling 2. Mathematical Properties of Max-min Rodeg Index

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Abstract. Recently, set of 148 discrete Adriatic indices has been defined. One of these indices is Max-min rodeg index. It is a good predictor of enthalpy of vaporization for octane isomers. It is also good predictor of standard enthalpy of vaporization for octane isomers and it has been shown that it is a good predictor of log water activity coefficient for polychlorobiphenyls. Tight mathematical bounds (expressed as the functions of the number of vertices) are analyzed for the following classes of graphs: connected graphs, trees, unicyclic graphs, chemical graphs, chemical trees, chemical unicyclic graphs and trees with prescribed number of pendant vertices. Further, we analyze maximal value of this index for graphs with maximal degree Δ and minimal value of this index for graphs with minimal degree *δ*. Also, we propose a series of open problems regarding mathematical properties of discrete Adriatic indices that have shown good predictive properties.

Keywords: molecular descriptor, extremal values, extremal graphs, chemical graphs, unicyclic graphs, trees

INTRODUCTION

One hundred and forty eight discrete Adriatic indices have been defined.[1] Also, QSAR and QSPR[2–4] studies of these indices have been preformed[1] on the benchmark sets[5] proposed by the International Academy of Mathematical Chemistry[6] in Ref. 1. Twenty of these indices have shown good predictive properties. One of these twenty indices is the Max-min rodeg index defined by:

$$Mm_{sde}(G) = \sum_{uv\in E(G)} \frac{\max\left\{\sqrt{d_u},\sqrt{d_v}\right\}}{\min\left\{\sqrt{d_u},\sqrt{d_v}\right\}} = \sum_{uv\in E(G)} \sqrt{\frac{\max\left\{d_u,d_v\right\}}{\min\left\{d_u,d_v\right\}}},$$

where $E(G)$ is the set of edges of G; and d_u and d_v are degrees of vertices u and v, respectively. This descriptor can be singled out as one of the most perspective Adriatic descriptors, because it gives three very good linear-model predictions: enthalpy of vaporization for octane isomers, standard enthalpy of vaporization for octane isomers and log water activity coefficient for polychlorobiphenyls. This is the reason why we study the mathematical properties of this very descriptor.

This index belongs to the large class of indices ϕ defined by:

$$\phi(G) = \sum_{uv\in E(G)} \alpha(d_u,d_v).$$

The most famous indices in this class are: the Randić connectivity index[7] defined by:

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

The Zagreb index[8] defined by:

$$M_2(G) = \sum_{uv\in E(G)} d_u d_v.$$

This index was modified to

$$^*M_2(G) = \sum_{uv\in E(G)} \frac{1}{d_u d_v}$$

and generalized to:[9]

$$^*M_2(G) = \sum_{uv\in E(G)} (d_u d_v)^{\lambda}.$$

Also note that each of the indices $\phi(G)=\sum_{uv\in E(G)}\alpha(d_u,d_v)$ can be reformulated to:

$$\phi(G)=\sum_{1\le i\le j\le\Delta}\alpha(i,j)\cdot m_{ij}(G),$$

Where $m_{ij}=m_{ij}(G)$ is the number of edges that are incident to vertices of degrees i and j. Especially:

$$Mm_{sde}(G)=\sum_{1\le i\le j\le\Delta}\sqrt{j/i}\cdot m_{ij}(G).$$

This reformulation is important, because values m_{ij} have been extensively studied.[10–20] In this paper we are interested in determining extremal values and extremal graphs of max-min rodeg index in several classes of graphs (with given number of vertices): the class of all connected graphs, the class of all trees, the class of all unycyclic graphs, the class of all chemical graphs, the class of all chemical trees, the class of all chemical unycyclic graphs, the class of all graphs with given maximal degree, the class of all graphs with given minimal degree, the class of all trees with given number of pendant vertices, the class of all connected graphs with given number of pendant vertices. We give some complete and some partial solutions of these problems.

MAIN RESULTS

Denote by $V(G)$ set of vertices in G. It is well known that:

Lemma 1. Let G be a graph with n vertices that does not have isolated vertices. Then

$$\sum_{uv\in E(G)}\left(\frac{1}{d_u}+\frac{1}{d_v}\right)=n$$

Proof: One has

$$\sum_{uv\in E(G)}\left(\frac{1}{d_u}+\frac{1}{d_v}\right)=\sum_{u\in V(G)}\sum_{v\in V(G):uv\in E(G)}\frac{1}{d_u}=\sum_{u\in V(G)}1=n.\ \blacksquare$$

Denote by n_i number of vertices of degree i. The following is also well known, but again proof is provided for the sake of the completeness of results:

Lemma 2. Let G be a tree with $n\ge 2$ vertices. Then G has at least two pendant vertices. Moreover, the only tree with exactly two pendant vertices is path.

Proof: From $n(G)=m(G)+1$, it follows that: $n_1(G)=\sum_{i=3}^{\Delta(G)}(i-2)n_i+2$ and this implies the Lemma. ■

Let us prove:

Theorem 1. Let G be a simple connected graph with $n\ge 2$ vertices and maximal degree Δ. Then,

$$Mm_{sde}(G)\le\frac{n\cdot\Delta}{2}.$$

Moreover, the equality holds if and only if G is Δ-regular graph.

Proof: Let us prove that

$$\frac{Mm_{sde}(G)}{n}\le\frac{\Delta}{2}$$

It holds:

$$Mm_{sde}(G)=\sum_{uv\in E(G)}\sqrt{\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}}=\frac{\sum_{uv\in E(G)}\sqrt{\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}}\cdot\left(\frac{1}{d_u}+\frac{1}{d_v}\right)}{\sum_{uv\in E(G)}\left(\frac{1}{d_u}+\frac{1}{d_v}\right)}=$$

$$\sum_{uv\in E(G)}\frac{1}{2}\max\{d_u,d_v\}\cdot\frac{\sqrt{\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}}}{\frac{1}{2}\left(1+\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}\right)}\cdot\left(\frac{1}{d_u}+\frac{1}{d_v}\right)$$

Hence, the ratio of $\sqrt{\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}}$ to $\frac{1}{2}\left(1+\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}\right)$ is just the ratio of geometric to arithmetic mean (of 1 and $\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}$). So, this ratio is ≤ 1, with equality if and only if $\frac{\max\{d_u,d_v\}}{\min\{d_u,d_v\}}=1$, or equivalently if and only if $d_u=d_v$. Thus

$$Mm_{sde}(G)\le\sum_{uv\in E(G)}\frac{1}{2}\max\{d_u,d_v\}\cdot\left(\frac{1}{d_u}+\frac{1}{d_v}\right)\le\frac{\Delta}{2}\sum_{uv\in E(G)}\left(\frac{1}{d_u}+\frac{1}{d_v}\right)=\frac{\Delta n}{2},$$

where the second inequality is equality if and only if every edge uv is such that that one of its vertices has degree Δ. Putting the conditions for equality in the two inequalities together, one sees that overall equality is achieved if and only if G is Δ regular. ■

Theorem 2. Let G be a simple connected graph with $n \geq 3$ vertices. Then

$$2\sqrt{2}+(n-3) \leq Mm_{sde}(G) \leq \frac{n(n-1)}{2}.$$

The equality in lower bound holds if and only if G is a path P_n with n vertices and the equality in the upper bound holds if and only if G is a complete graph K_n.

Proof: First, let us prove the lower bound. Distinguish two cases:

CASE 1: G is tree.
From Lemma 2, it follows that there are at least two edges incident to pendant vertices. Each of them can contribute at least $\sqrt{2/1}$. Each other edge contributes at least 1. Hence, $2\sqrt{2}+(n-3) \leq Mm_{sde}(G)$. Moreover, the equality implies that G has two pendant vertices, but this is possible only if $G = P_n$. It can be easily checked that $Mm_{sde}(P_n) = 2\sqrt{2}+(n-3)$.

CASE 2: G is not a tree.
G has at least n edges each of which contributes at least 1, hence

$$Mm_{sde}(G) \geq n > 2\sqrt{2}+(n-3).$$

Let us prove the upper bound. From the Theorem 1, it follows that:

$$Mm_{sde}(G) \leq \frac{n \cdot \Delta}{2} \leq \{\Delta \leq n-1\} \leq \frac{n(n-1)}{2}.$$

Moreover, equality holds if and only if G is $(n-1)$-regular graph, but the only such graph is the complete graph K_n.

Theorem 3. Let G be a tree with $n \geq 3$ vertices. Then

$$2\sqrt{2}+(n-3) \leq Mm_{sde}(G) \leq (n-1)^{3/2}.$$

The equality in lower bound holds if and only if is a path P_n and the equality in the upper bound holds if and only if G is a star S_n.

Proof: Lower bound follows from the Theorem 2. In order to prove the upper bound it is sufficient to note that contribution of each edge is at most $\sqrt{n-1}$ (in case when end-vertices have degrees 1 and $n-1$ respectively). The only graph such graph is the star S_n. ■

Let A_n be a graph obtained from the star S_n by adding an edge that connects two leaves as presented in the Figure 1.

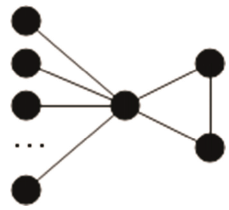

Figure 1. Graph A_n.

We shall need the following technical Lemma:

Lemma 3. Let $a \geq b \geq c > 0$ be real numbers. Then,

$$\sqrt{\frac{a}{b}}+\sqrt{\frac{b}{c}} \leq 1+\sqrt{\frac{a}{c}}$$

Proof: One has:

$$\left(\sqrt{a}-\sqrt{b}\right)\cdot\left(\sqrt{c}-\sqrt{b}\right) \leq 0$$
$$\sqrt{ac}-\sqrt{ab}-\sqrt{bc}+\sqrt{b^2} \leq 0$$
$$\sqrt{ac}+\sqrt{b^2} \leq \sqrt{bc}+\sqrt{ab}.$$

and division by bc yields the Theorem. ■

Let us prove:

Theorem 4. Let G be connected unicyclic graph with $n \geq 3$ vertices. Then

$$n \leq Mm_{sde}(G) \leq (n-3)\sqrt{n-1}+2\sqrt{\frac{n-1}{2}}+1.$$

Equality in the lower bound holds if and only if G is the cycle C_n and the equality in the upper bound holds if and only if G is the graph A_n.

Proof: Let us prove the lower bound. Note that contribution of each edge is at least 1, hence indeed $Mm_{sde}(G) \geq n$. The equality holds if and only if all edge contributes exactly 1; or equivalently each edge has end-vertices of the same degree. Hence, equality hold for regular uniciclyc graphs. Let d be a degree of all vertices in observed graph G. Then,

$$m(G) = n(G) \;\Rightarrow\; \frac{d \cdot n(G)}{2} = n(G) \;\Rightarrow\; d = 2.$$

The only connected 2-regular graph with n vertices is C_n.

Now, let us prove the upper bound. Let us distinguish 3 cases:

CASE 1: G has a vertex of degree $n-1$.
It can be verified that A_n is the only such graph with n vertices and that

$$Mm_{sde}\left(A_n\right)=\left(n-3\right)\sqrt{n-1}+2\sqrt{\frac{n-1}{2}}+1 .$$

CASE 2: G does not have a vertex of degree $n-1$ and it has a cycle of the length at least 4.
In this case the contribution of each edge in the cycle is at most $\sqrt{\frac{n-2}{2}}$ and the contribution of each other edge is at most $\sqrt{\frac{n-2}{1}}$, so that it is sufficient to prove that:

$$\left(n-4\right)\cdot\sqrt{n-2}+4\cdot\sqrt{\frac{n-2}{2}}<\left(n-3\right)\sqrt{n-1}+2\sqrt{\frac{n-1}{2}}+1;$$
$$\left(n-2\right)\cdot\sqrt{n-2}<\left(n-3+\sqrt{2}\right)\sqrt{n-1}+1,$$

and this is true, because $n-2<n-3+\sqrt{2}$ and $\sqrt{n-2}<\sqrt{n-1}$.

CASE 3: G does not have a vertex of degree $n-1$ and it has a cycle of length 3.
Denote by a,b and c the degrees of vertices in this cycle in such a way that $a\geq b\geq c$. It is sufficient to prove that:

$$\left(n-3\right)\cdot\sqrt{n-2}+\sqrt{\frac{a}{b}}+\sqrt{\frac{a}{c}}+\sqrt{\frac{b}{c}}<\left(n-3\right)\sqrt{n-1}+2\sqrt{\frac{n-1}{2}}+1.$$

Moreover, since $\sqrt{n-2}<\sqrt{n-1}$, it sufficient to prove that:

$$\sqrt{\frac{a}{b}}+\sqrt{\frac{a}{c}}+\sqrt{\frac{b}{c}}\leq 2\sqrt{\frac{n-1}{2}}+1.$$

Further, since the left hand-side is obviously increasing in a and decreasing in c, it is sufficient to prove that:

$$\sqrt{\frac{n-2}{b}}+\sqrt{\frac{n-2}{2}}+\sqrt{\frac{b}{2}}\leq 2\sqrt{\frac{n-1}{2}}+1.$$

Since, $\sqrt{\frac{n-2}{2}}\leq\sqrt{\frac{n-1}{2}}$, it is sufficient to prove that

$$\sqrt{\frac{n-2}{b}}+\sqrt{\frac{b}{2}}\leq\sqrt{\frac{n-2}{2}}+1.$$

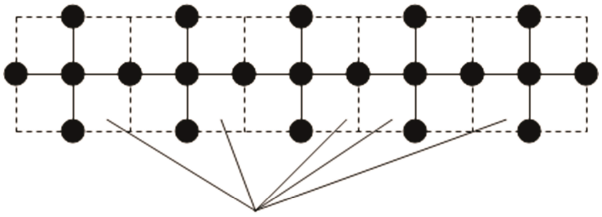

Figure 2. Graph B_n.

The last inequality follows from Lemma 3. ■

Theorem 5. Let G be a chemical connected graph with $n\geq 3$ vertices. Then

$$2\sqrt{2}+\left(n-3\right)\leq Mm_{sde}\left(G\right)\leq 2n .$$

The equality in the lower bound holds if and only if G is a path P_n, and the equality in the upper bound holds if and only if G is a 4-regular graph.

Proof: The lower bound follows directly from Theorem 2. The upper bound follows from Theorem 1. ■

Denoted by B_n, where $n\equiv 1$ (mod 4), the graph that is presented in the Figure 2.

Let us prove:

Theorem 6. Let G be a chemical tree with n vertices. Then

$$\left.\begin{cases} 0, & n=1 \\ 1, & n=2 \\ 2\sqrt{2}+\left(n-3\right), & n\geq 3\end{cases}\right\}\leq Mm_{sde}\left(G\right)\leq\left(1+\frac{\sqrt{2}}{2}\right)n+3-\frac{5}{2}\sqrt{2}$$

The equality in the lower bound holds if and only if G is a path P_n, and the equality in the upper bound holds for the graph in which each edge either connects vertices of degrees 1 and 4, or vertices of degrees 2 and 4 (the example of such graph is B_n).

Proof: The lower bound follows from Theorem 2. Let us prove the upper bound. If $n\leq 2$ the claim is trivial, hence we restrict our attention to graphs with at least three vertices. Let us denote:

$$\alpha\left(x,y\right)=\sqrt{\frac{\max\left\{d_x,d_y\right\}}{\min\left\{d_x,d_y\right\}}} .$$

Suppose to the contrary that there is a chemical tree G that contradicts the assumptions of the theorem. Denote by Γ_1 class of all such chemical trees. Let $G_1\in\Gamma_1$ be a tree with the smallest number of vertices of degree 3. Suppose that G_1 has at least one vertex of degree 3. Let

u be a vertex of degree 3 in G_1 and let u_1, u_2 and u_3 be its neighbors. Let G_1^+ be a graph obtained by adding one pendant vertex to u. Obviously, G_1^+ has a smaller number of vertices of degree 3 than G_1, so that:

$$Mm_{sde}\left(G_1^+\right) \leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_1\right)+1\right)+3-\frac{5}{2}\sqrt{2}.$$

Therefore:

$$Mm_{sde}\left(G_1^+\right)-Mm_{sde}\left(G_1\right) \leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_1\right)+1\right)+3-\frac{5}{2}\sqrt{2}- \left[\left(1+\frac{\sqrt{2}}{2}\right)n\left(G_1\right)+\left(3-\frac{5}{2}\sqrt{2}\right)\right]=1+\frac{\sqrt{2}}{2}$$

On the other hand, note that:

$$Mm_{sde}\left(G_1^+\right)-Mm_{sde}\left(G_1\right)=2+\sum_{i=1}^{3}\left[\alpha\left(4,d_{u_1}\right)-\alpha\left(3,d_{u_1}\right)\right].$$

Hence,

$$2+\sum_{i=1}^{3}\left[\alpha\left(4,d_{u_1}\right)-\alpha\left(3,d_{u_1}\right)\right]\leq 1+\frac{\sqrt{2}}{2}.$$

It can be easily checked that this holds if and only if $d_{u_1}=d_{u_2}=d_{u_3}=4$. Now, let G_1^i be a connected component of the graph G_1-u that contains vertex u_i, for each $i=1,...,3$. Let H_1^i be a graph obtained from G_1^i by adding to u_i one pendant vertex. It can be easily seen that:

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)-Mm_{sde}\left(G_1\right)= 3\cdot\sqrt{\frac{4}{1}}-3\cdot\sqrt{\frac{4}{3}}.$$

Hence,

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)= Mm_{sde}\left(G_1\right)+6-2\sqrt{3}$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\geq \left(1+\frac{\sqrt{2}}{2}\right)n\left(G_1\right)+9-2\sqrt{3}-\frac{5}{2}\sqrt{2} \quad (1)$$

On the other hand, note that each of graphs H_1^1, H_1^2 and H_1^3 has a smaller number of vertices of degree 3, than G_1. Hence,

$$Mm_{sde}\left(H_1^i\right)\leq\left(1+\frac{\sqrt{2}}{2}\right)n\left(H_1^i\right)+3-\frac{5}{2}\sqrt{2}.$$

Summing up the previous relation for $i=1,2,3$ we get:

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(H_1^1\right)+n\left(H_1^2\right)+n\left(H_1^3\right)\right)+3\cdot\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_1\right)+2\right)+3\cdot\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)n\left(G_1\right)+11-\frac{13}{2}\sqrt{2}$$

which is in contradiction with (1). Hence, we may conclude that G_1 has no vertices of degree 3.

Let Γ_2 be a class of graphs $G \in \Gamma_1$ without vertices of degree 3. Class Γ_2 is non-empty, because $G_1 \in \Gamma_2$. Let G_2 be a graph in the class Γ_2 with the smallest value of $m_{12}+m_{22}+m_{44}$. Let us distinguish 4 cases:

CASE 1: $m_{12}\left(G_2\right)\geq 1$.

Let G_2^- be graph obtained by contracting one edge that connects vertices of degrees 1 and 2. Note that

$$Mm_{sde}\left(G_2^-\right)\geq Mm_{sde}\left(G_2\right)-\sqrt{2}. \quad (2)$$

Since G_2^* has smaller value of $m_{12}+m_{22}+m_{44}$, it follows that:

$$Mm_{sde}\left(G_2^-\right)\leq\left(1+\frac{\sqrt{2}}{2}\right)n\left(G_2^-\right)+3-\frac{5}{2}\sqrt{2}= \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_2\right)-1\right)+3-\frac{5}{2}\sqrt{2}= \leq Mm_{sde}\left(G_2\right)-\left(1+\frac{\sqrt{2}}{2}\right),$$

which is in contradiction with (2).

CASE 2: $m_{22}(G_2) \geq 1$.

Let $G_2^{\#}$ be the graph obtained by contracting one edge that connects vertices of degrees 2. Note that

$$Mm_{sde}\left(G_2^{\#}\right) = Mm_{sde}\left(G_2\right) - 1. \qquad (3)$$

Since G_2^{-} has smaller value of $m_{12} + m_{22} + m_{44}$, it follows that:

$$Mm_{sde}\left(G_2^{\#}\right) \leq \left(1 + \frac{\sqrt{2}}{2}\right) n\left(G_2^{\#}\right) + 3 - \frac{5}{2}\sqrt{2} =$$
$$\left(1 + \frac{\sqrt{2}}{2}\right)\left(n\left(G_2\right) - 1\right) + 3 - \frac{5}{2}\sqrt{2} =$$
$$\leq Mm_{sde}\left(G_2\right) - \left(1 + \frac{\sqrt{2}}{2}\right),$$

which is in contradiction with (3).

CASE 3: $m_{44}(G_2) \geq 1$.

Let G_2^{+} be graph obtained by splitting one edge that connects vertices of degrees 4 in path of length 2. Note that

$$\begin{aligned} Mm_{sde}\left(G_2^{+}\right) &= Mm_{sde}\left(G_2\right) + 2 \cdot \sqrt{\frac{4}{2}} - 1 \cdot \sqrt{\frac{4}{4}} = \\ & Mm_{sde}\left(G_2\right) + 2 \cdot \sqrt{2} - 1. \end{aligned} \qquad (4)$$

Since G_2^{+} has smaller value of $m_{12} + m_{22} + m_{44}$, it follows that:

$$Mm_{sde}\left(G_2^{+}\right) \leq \left(1 + \frac{\sqrt{2}}{2}\right) n\left(G_2^{+}\right) + 3 - \frac{5}{2}\sqrt{2} =$$
$$\left(1 + \frac{\sqrt{2}}{2}\right)\left(n\left(G_2\right) + 1\right) + 3 - \frac{5}{2}\sqrt{2} =$$
$$\leq Mm_{sde}\left(G_2\right) + \left(1 + \frac{\sqrt{2}}{2}\right),$$

which is in contradiction with (4).

CASE 4: $m_{12}(G_2) + m_{22}(G_2) + m_{44}(G_2) = 0$.

In this case the only non-zero m_{ij} s are m_{14} and m_{24}. From Lemma 1, it follows that

$$\left(\frac{1}{1} + \frac{1}{4}\right) m_{14}\left(G_2\right) + \left(\frac{1}{2} + \frac{1}{4}\right) m_{24}\left(G_2\right) = n.$$

Since G_2 is tree, it follows that:

$$m_{14}\left(G_2\right) + m_{24}\left(G_2\right) = n - 1.$$

Solving this, we get:

$$m_{14}\left(G_2\right) = \frac{n+3}{2}$$

$$m_{24}\left(G_2\right) = \frac{n-5}{2}$$

Hence,

$$Mm_{sde}\left(G_2\right) = \frac{n+3}{2} \cdot 2 + \frac{n-5}{2} \cdot \sqrt{2} = \left(1 + \frac{\sqrt{2}}{2}\right) n + 3 - \frac{5}{2}\sqrt{2}.$$

All the cases are exhausted. It can be easily seen (by calculation analogous to that of Case 4) that every graph which every edge connects either edges of degrees 1 and 4, or edges of degrees 2 and 4 satisfies the equality. ■

Theorem 7. Let G be a chemical unicyclic graph with n vertices. Then

$$n \leq Mm_{sde}\left(G\right) \leq \left(1 + \frac{\sqrt{2}}{2}\right) n.$$

The equality in the lower bound holds if and only if G is a path P_n and the equality in the upper bound holds for the graph in which each edge either connects vertices of degrees 1 and 4, or vertices of degrees 2 and 4.

Proof: The lower bound follows from Theorem 3. Let us prove the upper bound. Denote $\alpha(x, y)$ as above. Suppose to the contrary that there is a unicyclic chemical graph G that contradicts the assumptions of the theorem. Denote by Γ_1 the class of all such unicyclic graphs. Let $G_1 \in \Gamma_1$ be a graph with the smallest number of vertices of degree 3. Suppose that G_1 has at least one vertex of degree 3. As above, let u be a vertex of degree 3 in G_1, and let u_1, u_2 and u_3 be its neighbors. Completely analogously as above, it can be shown that $d_{u_1} = d_{u_2} = d_{u_3} = 4$. Distinguish two cases:

CASE 1: Vertex u is not part of the unique cycle.

$G - u$ has three components one of which is a chemical unicyclic graph and two are chemical trees. Without loss of generality, we may assume that u_3 is contained in unicyclic component. Denote $G_1^1, G_1^2, G_1^3, H_1^1, H_1^2$ and H_1^3 as above. Completely analogously it can be shown that:

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)= Mm_{sde}\left(G_1\right)+6-2\sqrt{3}$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\geq \left(1+\frac{\sqrt{2}}{2}\right)n+6-2\sqrt{3} \tag{5}$$

On the other hand, note that H_1^1 and H_1^2 have smaller number of vertices of degree 3. Therefore,

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(H_1^1\right)+n\left(H_1^2\right)+n\left(H_1^3\right)\right)+2\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_1\right)+2\right)+2\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^1\right)+Mm_{sde}\left(H_1^2\right)+Mm_{sde}\left(H_1^3\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)n\left(G_1\right)+\left(8-4\sqrt{2}\right),$$

which is in contradiction with (5).

CASE 2: Vertex u is a part of the cycle.
$G-u$ has two components G_1^a and G_1^b both of which are chemical trees. Let H_1^a and H_1^b be obtained from G_1^a and G_1^b by adding one pendant vertex to each of the vertices u_1, u_2 and u_3. Similarly as above:

$$Mm_{sde}\left(H_1^a\right)+Mm_{sde}\left(H_1^b\right)=Mm_{sde}\left(G_1\right)+6-2\sqrt{3}. \tag{6}$$

On the other hand:

$$Mm_{sde}\left(H_1^a\right)+Mm_{sde}\left(H_1^b\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(H_1^a\right)+n\left(H_1^b\right)\right)+2\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^a\right)+Mm_{sde}\left(H_1^b\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)\left(n\left(G_1\right)+2\right)+2\left(3-\frac{5}{2}\sqrt{2}\right)$$

$$Mm_{sde}\left(H_1^a\right)+Mm_{sde}\left(H_1^b\right)\leq \left(1+\frac{\sqrt{2}}{2}\right)n\left(G_1\right)+\left(8-4\sqrt{2}\right),$$

which is in contradiction with (6). Hence, we may conclude that G_1 has no vertices of degree 3.

Let Γ_2 be a class of graphs $G\in\Gamma_1$ without vertices of degree 3. Class Γ_2 is non-empty, because $G_1\in\Gamma_2$. Let G_2 be a graph in the class Γ_2 with the smallest value of $m_{12}+m_{22}+m_{44}$. Let us distinguish 4 cases:

CASE 1: $m_{12}\left(G_2\right)\geq 1$.

CASE 2: $m_{22}\left(G_2\right)\geq 1$.

CASE 3: $m_{44}\left(G_2\right)\geq 1$.

These three cases can be proved completely analogously as above.

CASE 4: $m_{12}\left(G_2\right)+m_{22}\left(G_2\right)+m_{44}\left(G_2\right)=0$.

In this case the only non-zero m_{ij} s are m_{14} and m_{24}. From Lemma 1, it follows that

$$\left(\frac{1}{1}+\frac{1}{4}\right)m_{14}\left(G_2\right)+\left(\frac{1}{2}+\frac{1}{4}\right)m_{24}\left(G_2\right)=n.$$

Since G_2 is a unicyclic graph, it follows that:

$$m_{14}\left(G_2\right)+m_{24}\left(G_2\right)=n .$$

Solving this, we get:

$$m_{14}\left(G_2\right)=m_{24}\left(G_2\right)=\frac{n}{2}$$

Hence, $Mm_{sde}\left(G_2\right)=\frac{n}{2}\cdot 2+\frac{n}{2}\cdot\sqrt{2}=\left(1+\frac{\sqrt{2}}{2}\right)n.$ All the cases are exhausted.

It can be easily seen (by calculation analogous to that of Case 4) that every graph in which every edge connects either edges of degrees 1 and 4, or edges of degrees 2 and 4 satisfies the equality. ■

Theorem 8. Let G be a simple connected graph with $n\geq 2$ vertices and minimal degree δ. Then,

$$Mm_{sde}\left(G\right)\geq\frac{n\cdot\delta}{2}.$$

Moreover, the equality holds if and only if G is δ-regular graph.

Proof: Each edge contributes at least 1 and there are at least $\frac{n\cdot\delta}{2}$ edges. Obviously, equality holds only for δ-regular graphs. ■

We shall need the following technical Lemma:

Lemma 4. Function $f:\{3,4,5,...\}\to\mathbb{R}$ defined by

$$f(x)=\frac{\frac{\sqrt{x}}{2}+(x-1)\sqrt{x}-x}{x-2}$$

is a strictly increasing function.

Proof: Note that $f(3)\approx 1.33$ and $f(4)=1.5$, hence indeed $f(3)<f(4)$. It is sufficient to prove that function $g:[4,+\infty)\to\mathbb{R}$ defined by

$$g(x)=\frac{\frac{\sqrt{x}}{2}+(x-1)\sqrt{x}-x}{x-2}$$

is an increasing function, *i.e.* that its first derivative is positive. Now,

$$g'(x)=\frac{2+8\sqrt{x}-11x+2x^2}{4(x-2)\sqrt{x}}.$$

Denominator is positive, whence it is sufficient to prove that

$$2+8\sqrt{x}-11x+2x^2\geq 0.$$

Let us prove this. Note that $\frac{4\sqrt{x}+x^2}{2}\geq\sqrt{4x^{5/2}}$, because it is inequality of arithmetic and gemometric mean, whence

$$2+8\sqrt{x}-11x+2x^2=2-11x+4\cdot\frac{4\sqrt{x}+x^2}{2}\geq$$
$$2-11x+4\cdot\sqrt{4x^{5/2}}=2-11x+8x^{5/4}.$$

It is sufficient to show that $8x^{5/4}\geq 11x$, but this is equivalent to $x\geq\left(\frac{11}{8}\right)^4$ which holds for $x\in[0,4]$. ■

Let us prove:

Theorem 9. Let G be a tree with n vertices and $k\geq 2$ pendant vertices. Then,

$$\left\{\begin{array}{ll} n-3+2\sqrt{2}, & k=2 \\ (n-1)+\left(\sqrt{2}+\sqrt{\frac{3}{2}}-2\right)k, & k\geq 3\end{array}\right\}\leq Mm_{sde}(G)\leq$$
$$(k-1)\cdot\sqrt{k}+\sqrt{\frac{k}{2}}+\sqrt{2}+n-k-2.$$

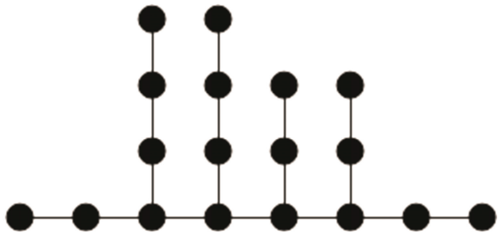

Figure 3. The extremal graph for the lower bound.

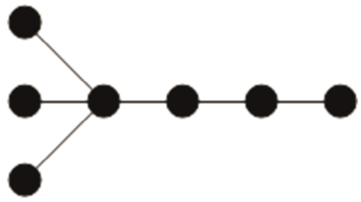

Figure 4. Graph $S_{7,4}$.

The inequality on the left hand-side is an equality if and only if the graph G is a path or G is obtained from a graph H consisting solely of vertices of degrees 1 and 3; via a process where each edge connecting vertices of degrees 1 and 3 is replaced by a path of length at least 2. The inequality on the right-hand side is equality if and only if the graph G is graph $S_{n,k}$ obtained from star S_{k+1} by replacing one of its edges by a path of length $n-k$.

Before proving this theorem, let us give the following two remarks:

Remark 1. Note that the extremal graph for the upper bound is unique (up to isomorphism) while for lower bound there can be many extremal graphs. Let us illustrate the extremal graphs by the following examples:

1) the example of the extremal graph for the lower bound in the case of $n=18$ and $k=6$ is presented on the Figure 3.

2) the extremal graph $S_{7,4}$ is given by the Figure 4.

Remark 2. Note that extremal graph for the lower bound exists only if $k\leq 2+\frac{n-4}{3}=\frac{n+2}{3}$. Hence, in the case $k>\frac{n+2}{3}$, it is possible to improve the upper bound. Here, we propose as an open problem to find a sharp upper bound for all values of n and k.

Proof of Theorem 9: First, let us prove the lower bound. Suppose that there is a graph G which contradicts the assumption of the Theorem. Denote by $u_1,u_2,...,u_k$ pendant vertices of G. Let E_i be the set of edges from u_i to the first vertex of degree greater than 2. Denote this vertex by v_i. It can be easily seen that

$E_i \cap E_j = \varnothing$ for each $1 \le i < j \le k$. Let $E_0 = E(G) \setminus \left(\bigcup_{i=1}^{k} E_i \right)$. Sets $E_0, E_1, ..., E_k$ form a partition of $E(G)$. Let us prove that:

Claim A. $\sum_{uv \in E_0(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}} \ge |E_0|$ with equality if and only if all edges connect vertices of the same degree.

Proof: Just note that contribution of each edge is at least 1. ■

Claim B. Let $i = 1, ..., k$, then $\sum_{uv \in E_i(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}} \ge |E_i| + \sqrt{2} + \sqrt{\frac{3}{2}} - 2$ with equality if and only if $d_{v_i} = 3$ and $|E_i| > 1$.

Proof: If $|E_i| = 1$, then

$$\sum_{uv \in E_i(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}} = \sqrt{\frac{d_{v_i}}{d_{u_i}}} =$$

$$\sqrt{d_{v_i}} \ge \sqrt{3} > \sqrt{2} + \sqrt{\frac{3}{2}} - 1 = |E_i| + \sqrt{2} + \sqrt{\frac{3}{2}} - 2$$

If $|E_i| > 1$ then,

$$\sum_{uv \in E_i(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}} = \sqrt{\frac{d_{v_i}}{2}} + \sqrt{2} + |E_i| - 2 \ge$$

$$|E_i| + \sqrt{2} + \sqrt{\frac{3}{2}} - 2$$

and equality holds if and only if $d_{v_i} = 3$. ■

From Claims A and B, it follows that

$$\sum_{uv \in E_i(G)} \sqrt{\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}} \ge |E_0| + \sum_{i=1}^{k} \left(|E_i| + \sqrt{2} + \sqrt{\frac{3}{2}} - 2 \right) =$$

$$\sum_{i=0}^{k} |E_i| + \left(\sqrt{2} + \sqrt{\frac{3}{2}} - 2 \right) k = (n-1) + \left(\sqrt{2} + \sqrt{\frac{3}{2}} - 2 \right) k.$$

Moreover, equality holds only if $d_{v_i} = 3$ and $|E_i| > 1$ for each $i = 1, ..., k$; and a (connected) graph induced by edges in E_0 is regular. This is equivalent to the fact that G is an extremal graph described in the theorem.

Now, let us prove the upper bound. If $k \le 2$, the claim is trivial. Hence, suppose that $k \ge 3$. Let us prove the following claims:

Claim C. Let G be graph with maximal value of $Mm_{sde}(G)$ among all graphs with n vertices. If G has two vertices of degree greater than 2, then each vertex of degree 1 is adjacent to vertex of degree greater than 2.

Proof: Suppose to the contrary. Let u_1 be a vertex of degree 1, u_2 its neighbor of degree 2 and u_3 the other neighbor of u_2. Let v_1 and v_2 be two vertices of degree greater than 2 (possibly u_3 can be one of vertices v_1 and v_2). Denote by w a vertex adjacent to v_1 in the path from v_1 to v_2. Let G' be a graph such that:

$$V(G') = V(G);$$
$$E(G') = E(G) \setminus \{u_1u_2, u_2u_3, v_1w\} \cup \{u_1u_3, v_1u_2, u_2w\}.$$

Note that degrees of all vertices in G and G' are the same. Hence,

$$Mm_{sde}(G') - Mm_{sde}(G') =$$

$$\sqrt{\frac{d_{u_3}}{d_{u_1}}} + \sqrt{\frac{d_{v_1}}{d_{u_2}}} + \sqrt{\frac{d_w}{d_{u_2}}} - \sqrt{\frac{d_{u_2}}{d_{u_1}}} - \sqrt{\frac{d_{u_3}}{d_{u_2}}} - \sqrt{\frac{\max\{d_{v_1}, d_w\}}{\min\{d_{v_1}, d_w\}}} =$$

$$= \left(\sqrt{d_{u_3}} - \sqrt{2} - \sqrt{\frac{d_{u_3}}{2}} + 1 \right) +$$

$$\left(\sqrt{\frac{d_{v_1}}{2}} + \sqrt{\frac{d_w}{2}} - \sqrt{\frac{\max\{d_{v_1}, d_w\}}{\min\{d_{v_1}, d_w\}}} - 1 \right).$$

Lemma 3 implies that the first bracket is non-negative. Hence, In order to obtain a contradiction, it is sufficient to prove that the second bracket is positive. Denote $x = \max\{d_{v_1}, d_w\}$ and $y = \min\{d_{v_1}, d_w\}$. We need to prove that:

$$\sqrt{\frac{x}{2}} + \sqrt{\frac{y}{2}} \ge \sqrt{\frac{x}{y}} + 1.$$

Since, $x, y > 3$, it follows that $\sqrt{\frac{x}{2}} > \sqrt{\frac{x}{y}}$ and $\sqrt{\frac{y}{2}} > 1$, which proves the claim. ■

Claim D. Let G be graph with maximal value of $Mm_{sde}(G)$ among observed graphs and such that:

$$Mm_{sde}(G) \ge (k-1) \cdot \sqrt{k} + \sqrt{\frac{k}{2}} + \sqrt{2} + n - k - 2$$

Then, there is exactly one vertex in G of degree greater than 2.

Proof: Since $k \geq 3$, G has at least one vertex of degree greater than 2. Suppose to the contrary that G has at least two vertices of degree greater than 2. From $m(G) = n(G) - 1$, it follows that $k = n_1(G) = \sum_{i=3}^{\Delta} n_i(G)(i-2) + 2$. Hence, $\Delta < k$. Denote as above

$$\alpha(x,y) = \sqrt{\frac{\max\{x,y\}}{\min\{x,y\}}}.$$

In order to obtain a contradiction, we need to prove that:

$$\sum_{uv \in E(G)} \alpha(d_u, d_v) < (k-1)\cdot\sqrt{k} + \sqrt{\frac{k}{2}} + \sqrt{2} + n - k - 2$$

$$\sum_{uv \in E(G)} \left(\alpha(d_u, d_v) - 1\right) < (k-1)\cdot\sqrt{k} + \sqrt{\frac{k}{2}} - k + \left(\sqrt{2} - 1\right). \quad (7)$$

Let us denote different sets of edges of G, thusly: E_{i+} for those edges that connect vertex of degrees $i = 1,2$ to one of degree; E_{22} for those connecting two vertices of degree 2; and E_{++} for those connecting vertices both of which have degrees > 2. Then, from the Claim C, it follows that $E = E_{1+} \cup E_{22} \cup E_{2+} \cup E_{++}$. Analogously as in the proof of the Claim C, it can be shown that

$$\alpha(x,y) \leq \alpha(x,2) + \alpha(y,2) - 1$$

holds for each edge uv in E_{++}. Therefore:

$$\begin{aligned}
&\sum_{uv \in E(G)} \left(\alpha(d_u,d_v) - 1\right) = \\
&\sum_{uv \in E_{1+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \sum_{uv \in E_{22}(G)} \left(\alpha(d_u,d_v) - 1\right) + \\
&\sum_{uv \in E_{2+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \sum_{uv \in E_{++}(G)} \left(\alpha(d_u,d_v) - 1\right) = \\
&\sum_{uv \in E_{1+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \sum_{uv \in E_{2+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \\
&\sum_{uv \in E_{++}(G)} \left(\alpha(d_u,d_v) - 1\right) \leq \\
&\sum_{uv \in E_{1+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \sum_{uv \in E_{2+}(G)} \left(\alpha(d_u,d_v) - 1\right) + \\
&\sum_{uv \in E_{++}(G)} \left(\alpha(d_u,2) + \alpha(d_v,2) - 2\right) = \\
&= \sum_{u \in V(G): d_u \geq 3} \left(\sum_{\substack{v \in V(G): uv \in E(G) \\ \text{and } d_v \geq 2}} \left(\alpha(d_u,2) - 1\right) + \sum_{\substack{v \in V(G): uv \in E(G) \\ \text{and } d_v = 1}} \left(\alpha(d_u,1) - 1\right) \right) \leq \\
&\leq \sum_{u \in V(G): d_u \geq 3} \left(\left(\alpha(d_u,2) - 1\right) + (d_u - 1)\left(\alpha(d_u,1) - 1\right) \right) \leq \\
&\sum_{u \in V(G): d_u \geq 3} \left(\sqrt{\frac{d_u}{2}} + (d_u - 1)\sqrt{d_u} - d_u \right).
\end{aligned}$$

Hence, in order to prove (7), it is sufficient to prove:

$$\sum_{u \in V(G): d_u \geq 3} \left(\sqrt{\frac{d_u}{2}} + (d_u - 1)\sqrt{d_u} - d_u \right) < (k-1)\cdot\sqrt{k} + \sqrt{\frac{k}{2}} - k + \left(\sqrt{2} - 1\right). \quad (8)$$

From $n(G) = m(G) + 1$, it follows that $k = n_1(G) = \sum_{k \geq 3}^{\Delta} \left(n_i(G) - 2\right) + 2$, *i.e.* $k - 2 = \sum_{u \in V(G): d_u \geq 3} (d_u - 2)$

Hence, in order to prove (8), it is sufficient to prove that:

$$\frac{\sum_{u \in V(G): d_u \geq 3} \left(\sqrt{\frac{d_u}{2}} + (d_u - 1)\sqrt{d_u} - d_u \right)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} < \frac{(k-1)\cdot\sqrt{k} + \sqrt{\frac{k}{2}} - k + \left(\sqrt{2} - 1\right)}{k - 2}$$

Let us prove this. Let function f be defined as in Lemma 4. Then,

$$\begin{aligned}
&\frac{\sum_{u \in V(G): d_u \geq 3} \left(\sqrt{\frac{d_u}{2}} + (d_u - 1)\sqrt{d_u} - d_u \right)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} = \\
&\frac{\sum_{u \in V(G): d_u \geq 3} \left(\frac{\sqrt{\frac{d_u}{2}} + (d_u - 1)\sqrt{d_u} - d_u}{d_u - 2} (d_u - 2) \right)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} = \\
&= \frac{\sum_{u \in V(G): d_u \geq 3} \left(f(d_u)(d_u - 2) \right)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} \leq \frac{\sum_{u \in V(G): d_u \geq 3} \left(f(\Delta)(d_u - 2) \right)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} = \\
&f(\Delta) \cdot \frac{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)}{\sum_{u \in V(G): d_u \geq 3} (d_u - 2)} < f(\Delta) < f(k) =
\end{aligned}$$

$$\frac{(k-1)\cdot\sqrt{k}+\sqrt{\frac{k}{2}}-k}{k-2}<\frac{(k-1)\cdot\sqrt{k}+\sqrt{\frac{k}{2}}-k+\left(\sqrt{2}-1\right)}{k-2}.$$

This proves the claim. ■

Hence, we may assume that graph G has exactly one vertex v of degree greater than 2. Since G has exactly k pendant vertices, it follows that $d_v = k$ and vertex v is adjacent to k pendant paths. Let x be number of pendant vertices incident to x (then, $k-x$ pendant path have length at least 2). Then,

$$\sum_{uv\in E(G)}\left(\alpha(x,y)-1\right)=x\cdot\left(\sqrt{k}-1\right)+(k-x)\cdot\left(\sqrt{\frac{k}{2}}+\sqrt{2}-2\right)$$

$$\sum_{uv\in E(G)}\alpha(x,y)=x\cdot\left(\sqrt{k}-1\right)+(k-x)\cdot\left(\sqrt{\frac{k}{2}}+\sqrt{2}-2\right)+n-1$$

From Lemma 3, it follows that $\sqrt{k}-1>\sqrt{\frac{k}{2}}+\sqrt{2}-2$, hence the maximum is indeed obtained for the graph $S_{n,k}$. It can be easily checked that:

$$Mm_{sde}\left(S_{n,k}\right)=(k-1)\cdot\sqrt{k}+\sqrt{\frac{k}{2}}+\sqrt{2}+n-k-2 .$$

This proves the Theorem. ■

CONCLUSIONS AND OPEN PROBLEMS

In this paper we have analyzed the Max-min rodeg index defined by: $Mm_{sde}(G)=\sum_{uv\in E(G)}\frac{\max\left\{\sqrt{d_u},\sqrt{d_v}\right\}}{\min\left\{\sqrt{d_u},\sqrt{d_v}\right\}}$.

We have studied extremal values and extremal graphs of the max-min rodeg index in several classes of graphs (with given number of vertices):

1) the class of all connected graphs
2) the class of all trees
3) the class of all unycyclic graphs
4) the class of all chemical graphs
5) the class of all chemical trees
6) the class of all chemical unycyclic graphs
7) the class of all graphs with given maximal degree
8) the class of all graphs with given minimal degree
9) the class of all trees with given number of pendant vertices
10) the class of all connected graphs with given number of pendant vertices.

We gave some complete and some partial solutions of problems 1)-9) and we have left 10) as an open problem.

Here, we propose the following open problems which solution would make the study of Max-min rodeg index more complete:

a) Find extremal values of $Mm_{sde}(G)$ where G is connected graph with n vertices and k pendant edges;
b) Find minimal values of $Mm_{sde}(G)$ where G is a tree n vertices and k pendant edges where $k>\frac{n+2}{3}$;
c) Find minimal value of $Mm_{sde}(G)$ where G is connected graph with n vertices and maximal degree Δ;
d) Find maximal value of $Mm_{sde}(G)$ where G is connected graph with n vertices and minimal degree δ.

Also, it would be of interest to analyze classes of graphs 1)-10) for the remaining 19 discrete Adriatic indices found important in paper.[1] Namely, for the indices:

- Randić type lodeg index: $\sum_{uv\in E(G)}\ln(d_u)\cdot\ln(d_v)$;
- Randić type sdi index: $\sum_{uv\in E(G)}\left(D_x^2 D_y^2\right)$;
- Randić type hadi index: $\sum_{uv\in E(G)}0.5^{D_u}\cdot 0.5^{D_v}=\sum_{uv\in E(G)}\frac{1}{2^{D_u+D_v}}$;
- sum lordeg index: $\sum_{uv\in E(G)}\left(\sqrt{\ln d_x}+\sqrt{\ln d_y}\right)=\sum_{v\in V(G)}d_x\sqrt{\ln d_x}$;
- inverse sum lordeg index: $\sum_{uv\in E(G)}\frac{1}{\sqrt{\ln(d_u)}+\sqrt{\ln(d_v)}}$;
- inverse sum indeg: $\sum_{uv\in E(G)}\frac{1}{\frac{1}{d_u}+\frac{1}{v_v}}=\sum_{uv\in E(G)}\frac{d_u d_v}{d_u+d_v}$;
- misbalance lodeg index: $\sum_{uv\in E(G)}\left|\ln d_u-\ln d_v\right|$;
- misbalance losdeg index: $\sum_{uv\in E(G)}\left|\ln^2 d_u-\ln^2 d_v\right|$;
- misbalance indeg index: $\sum_{uv\in E(G)}\left|\frac{1}{d_u}-\frac{1}{d_v}\right|$;

- misbalance irdeg index: $\sum_{uv\in E(G)} \left| \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right|$;
- misbalance rodeg index: $\sum_{uv\in E(G)} \left| \sqrt{d_u} - \sqrt{d_v} \right|$;
- misbalance deg index: $\sum_{uv\in E(G)} \left| d_u - d_v \right|$;
- misbalance hadeg index:
$$\sum_{uv\in E(G)} \left| \left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v} \right| = \sum_{uv\in E(G)} \left| 2^{-d_u} - 2^{-d_v} \right|;$$
- misbalance indi index: $\sum_{uv\in E(G)} \left| \frac{1}{D_u} - \frac{1}{D_v} \right|$;
- min-max rodeg index:
$$\sum_{uv\in E(G)} \frac{\min\left\{\sqrt{d_u}, \sqrt{d_v}\right\}}{\max\left\{\sqrt{d_u}, \sqrt{d_v}\right\}} = \sum_{uv\in E(G)} \sqrt{\frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}}};$$
- min-max sdi index:
$$\sum_{uv\in E(G)} \frac{\min\left\{D_u^{\,2}, D_v^{\,2}\right\}}{\max\left\{D_u^{\,2}, D_v^{\,2}\right\}} = \sum_{uv\in E(G)} \left(\frac{\min\{D_u, D_v\}}{\max\{D_u, D_v\}}\right)^2;$$
- max-min deg index: $\sum_{uv\in E(G)} \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}$;
- max-min sdeg index:
$$\sum_{uv\in E(G)} \frac{\max\left\{d_u^2, d_v^2\right\}}{\min\left\{d_u^2, d_v^2\right\}} = \sum_{uv\in E(G)} \left(\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}}\right)^2;$$
- symmetric division deg index:
$$\sum_{uv\in E(G)} \left(\frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}} + \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} \right).$$

Hence, 19 descriptors are given, 10 classes of graphs are given, and in each case we are interested in (sharp) lower and upper bound. This gives the total of 380 open problems. Solving these problems would be an important contribution to the mathematical theory of chemically relevant discrete Adriatic indices.

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SAŽETAK

Vezno-aditivno modeliranje 2. Matematička svojstva max-min Rodegovog indeksa

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Nedavno je skup od 148 Jadranskih indeksa (Adriatic indices) definiran. Max-min rodeg indeks je jedan od ovih indeksa. Pokazano je da je ovaj indeks dobar prediktor entalpije vaporizacije i standardne entalpije vaporizacije za izomere oktana. Također je pokazano da je dobar prediktor logaritma koeficijenta vodene aktivnosti za poliklorobifenile. Stroge gornje i donje međe (iskazane u terminima broja vrhova) su analizirane za sljedeće familije grafova: povezani grafovi, stabla, uniciklički grafovi, kemijski grafovi, kemijska stabla, kemijski uniciklički grafovi, te stabla s propisanim brojem listova. Nadalje, istraživana su maksimalna vrijednost ovog indeksa za grafove maksimalnog stupnja Δ, te minimalna vrijednost za grafove minimalnog stupnja *δ*. Također je dan i niz otvorenih problema o diskretnim jadranskim indeksima koji imaju dobra predikcijska svojstva.