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Exponential Vertex–Degree–Based Topological Indices and Discrimination

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Abstract

We discuss the discrimination property of vertex–degree–based (VDB) topological indices over $\mathcal{G}_n$, the set of graphs with n non-isolated vertices. Concretely, we consider a partition of $\mathcal{G}_n$ into equivalence classes induced by an equivalence relation on $\mathcal{G}_n$. Then we say that a VDB topological index has the discrimination property with respect to an equivalence relation on $\mathcal{G}_n$ if it discriminates equivalence classes. This is a generalization of the usual concept of discrimination in topological indices. If φ is a VDB topological index, then we introduce the $\widehat{m}_{\varphi}$-structure relation on $\mathcal{G}_n$ and show that the exponential of the best known VDB topological indices have the discrimination property. In view of the nice mathematical properties e^{φ} has, we study extremal values of Randić's exponential index over $\mathcal{G}_n$.

1 Introduction

In the chemical literature, a large number of molecular structure descriptors (topological indices) have been considered for studying correlations between the structure of a molecular compound and its physico-chemical properties or biological activity (QSPR/QSAR) [5, 24, 25]. One special category are the vertex–degree–based (VDB for short) topological indices, which are defined in terms of the degree of the vertices of the (molecular) graph [2, 6, 9, 12, 13, 21]. Some of the best known VDB topological indices are listed in Table 1.

Index	Notation	φ_{ij}
First Zagreb [10]	$\mathcal{FZ}$	$i+j$
Second Zagreb [10]	$\mathcal{SZ}$	ij
Randić [23]	χ	$\frac{1}{\sqrt{ij}}$
Harmonic [28]	$\mathcal{H}$	$\frac{2}{i+j}$
Geometric-Arithmetic [26]	$\mathcal{GA}$	$\frac{2\sqrt{ij}}{i+j}$
Sum-Connectivity [27]	$\mathcal{SC}$	$\frac{1}{\sqrt{i+j}}$
Atom-Bond-Connectivity [7]	$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$
Augmented Zagreb [8]	$\mathcal{AZ}$	$\left(\frac{ij}{i+j-2}\right)^3$

Table 1. Some well-known VDB topological indices.

Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. Recently in [22], the VDB topological indices over $\mathcal{G}_n$ were identified with vectors in $\mathbb{R}^h$, where $h = \frac{(n-1)n}{2}$. More precisely, we order lexicographically the elements of

$$K = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leq i \leq j \leq n-1\},$$

as

$$\begin{array}{ccccccccccc} (1,1) & < & (1,2) & < & (1,3) & < & (1,4) & < & \cdots & & < & (1,n-1) \\ & < & (2,2) & < & (2,3) & < & (2,4) & < & \cdots & & < & (2,n-1) \\ & & & < & (3,3) & < & (3,4) & < & \cdots & & < & (3,n-1) \\ & & & & & & & & \vdots & \vdots & \vdots & \vdots \\ & & & & & & & & < & (n-2,n-2) & < & (n-2,n-1) \\ & & & & & & & & & & < & (n-1,n-1)\,. \end{array}$$

Consequently, we can express every vector of $\mathbb{R}^h$ as (φ_{ij}), where $\varphi_{ij} \in \mathbb{R}$ for all $(i,j) \in K$. Consider the function $m : \mathcal{G}_n \longrightarrow \mathbb{R}^h$ defined by $m(G) = (m_{ij}(G))_{(i,j)\in K}$, where $G \in \mathcal{G}_n$. Formally, a VDB topological index is a function $T_\varphi : \mathcal{G}_n \longrightarrow \mathbb{R}$ defined as

$$T_\varphi(G) = m(G) \cdot \varphi, \tag{1}$$

for all $G \in \mathcal{G}_n$, where $\varphi \in \mathbb{R}^h$ and "$\cdot$" denotes the dot product over $\mathbb{R}^h$. In view of (1), we identify VDB topological indices over $\mathcal{G}_n$ with vectors in $\mathbb{R}^h$, and simplified the notation, writing $\varphi(G)$ instead of $T_\varphi(G)$: if $\varphi \in \mathbb{R}^h$ then for every $G \in \mathcal{G}_n$

$$\varphi(G) = m(G) \cdot \varphi. \tag{2}$$

In this paper we discuss the discrimination property of VDB topological indices over $\mathcal{G}_n$. Concretely, in Section 2 we consider a partition of $\mathcal{G}_n$ into equivalence classes induced by an equivalence relation on $\mathcal{G}_n$. Then if $\varphi \in \mathbb{R}^h$ we say that φ has the discrimination property with respect to an equivalence relation on $\mathcal{G}_n$ if it discriminates equivalence classes (Definition 2.1). This is a generalization of the usual concept of discrimination in topological indices. The discrimination power of graphs has been investigated extensively [3, 4, 16].

In Definition 2.3 we introduce the $\widehat{m}_\varphi$-structure relation over $\mathcal{G}_n$. Although the VDB topological indices φ listed in Table 1 do not have the discrimination property with respect to the $\widehat{m}_\varphi$-relation on $\mathcal{G}_n$, we show in Theorem 3.4, based on the classical Lindemann-Weierstrass's Theorem on algebraic numbers, that the exponentials e^φ do have the discrimination property with respect to the $\widehat{m}_\varphi$-relation on $\mathcal{G}_n$.

In view of the nice mathematical properties the exponentials e^φ have, in Section 4 we study the extremal values of Randić's exponential index over $\mathcal{G}_n$. We show in Theorem 4.3 that the star S_n attains the minimal value and the complete graph K_n attains the maximal value. We note that the Randić index is perhaps the topological index most frequently used QSPR/QSAR studies [14, 15]. For surveys of its mathematical properties we refer to [11, 17–19]. Discrimination properties of the Randić index were considered in [20].

2 Discrimination of VDB topological indices

Let us recall that a relation "$\sim$" on $\mathcal{G}_n$ is an equivalence relation if it is reflexive, symmetric and transitive. Let $G \in \mathcal{G}_n$ and denote $[G] = \{H \in \mathcal{G}_n : G \sim H\}$ the equivalence class of G. Then the distinct equivalence classes with respect to "$\sim$" determine a partition of $\mathcal{G}_n$.

Definition 2.1 *Let $\varphi \in \mathbb{R}^h$ and "$\sim$" an equivalence relation on $\mathcal{G}_n$. We say that the φ has the discrimination property with respect to "$\sim$" if it satisfies the following condition: for all $G, G' \in \mathcal{G}_n$*

$$\varphi(G) = \varphi(G') \Longleftrightarrow G \sim G'.$$

In other words, φ has the discrimination property with respect to an equivalence relation on $\mathcal{G}_n$ if it discriminates equivalence classes. Note that if the equivalence relation on $\mathcal{G}_n$ is isomorphism of graphs "$\cong$", then we obtain the usual concept of discrimination: for all $G, G' \in \mathcal{G}_n$

$$\varphi(G) = \varphi(G') \Longleftrightarrow G \cong G'.$$

But there are other equivalence relations on $\mathcal{G}_n$ which are interesting.

Example 2.2 *We say that two graphs G and G' of $\mathcal{G}_n$ have the same m-structure if $m(G) = m(G')$. Clearly, this is an equivalence relation on $\mathcal{G}_n$. If $\varphi \in \mathbb{R}^h$ then it follows easily by (2) that if $m(G) = m(G')$ then $\varphi(G) = \varphi(G')$. However, the Randić index $\chi = \left(\frac{1}{\sqrt{ij}}\right) \in \mathbb{R}^h$ has not the discrimination property with respect to the m-structure relation because $\chi(G) = \frac{n}{2}$ for all regular graphs $G \in \mathcal{G}_n$. Consequently, there exists graphs in $\mathcal{G}_n$ with different m-structure but equal Randić index.*

Let us define coarser relations than the m-structure on $\mathcal{G}_n$. Let $\varphi = (\varphi_{ij}) \in \mathbb{R}^h$. We define an equivalence relation over K: if $(i,j), (i',j') \in K$ then

$$(i,j) \sim (i',j') \text{ if and only if } \varphi_{ij} = \varphi_{i'j'}. \tag{3}$$

Let $[i,j]$ denote the equivalence class of $(i,j) \in K$. Let

$$[i_1, j_1], [i_2, j_2], \ldots, [i_p, j_p], \tag{4}$$

be the distinct equivalence classes that form a partition on K. We may assume that the representative chosen in each class is the least element of the class (with respect to the order in K) and that

$$(i_1, j_1) < (i_2, j_2) < \cdots < (i_p, j_p).$$

Consider the vector of $\mathbb{R}^p$

$$\widehat{\varphi} = (\varphi_{i_k j_k})_{k=1,\ldots,p}. \tag{5}$$

On the other hand, for each $G \in \mathcal{G}_n$ we define for each $k = 1, \ldots, p$

$$\widehat{m}_{i_k j_k}(G) = \sum_{(r,s)\in[i_k,j_k]} m_{rs}(G).$$

Now consider the vector of $\mathbb{R}^p$

$$\widehat{m}_\varphi(G) = (\widehat{m}_{i_k j_k}(G))_{k=1,\ldots,p}. \tag{6}$$

Definition 2.3 *Let $\varphi \in \mathbb{R}^h$ and $G, G' \in \mathcal{G}_n$. We say that G and G' have the same $\widehat{m}_\varphi$-structure if and only if $\widehat{m}_\varphi(G) = \widehat{m}_\varphi(G')$.*

The $\widehat{m}_\varphi$-structure relation on $\mathcal{G}_n$ is clearly an equivalence relation. Moreover, for all $G, G' \in \mathcal{G}_n$, if $\varphi \in \mathbb{R}^h$ then

$$G \cong G' \Longrightarrow m(G) = m(G') \Longrightarrow \widehat{m}_\varphi(G) = \widehat{m}_\varphi(G').$$

Consequently, the $\widehat{m}_\varphi$-structure relation on $\mathcal{G}_n$ is coarser than both the m-structure relation and the isomorphism relation on $\mathcal{G}_n$.

Example 2.4 *Let $n = 5$ so that $h = 10$. Then K is ordered as*

$$\begin{array}{ccccccc} (1,1) & < & (1,2) & < & (1,3) & < & (1,4) \\ & < & (2,2) & < & (2,3) & < & (2,4) \\ & & & < & (3,3) & < & (3,4) \\ & & & & & < & (4,4)\,. \end{array}$$

1. *Consider the Randić index $\chi = \left(\frac{1}{\sqrt{ij}}\right) \in \mathbb{R}^{10}$. The partition on K induced by χ is*

   $$[1,1] < [1,2] < [1,3] < [1,4] < [2,3] < [2,4] < [3,3] < [3,4] < [4,4]\,.$$

   Note that $(2,2) \in [1,4]$. In this case $p = 9$ and for $G \in \mathcal{G}_5$,

   $$\widehat{m}_\chi(G) = (m_{11}, m_{12}, m_{13}, m_{14} + m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})^\top \in \mathbb{R}^9,$$

   where $m_{ij} = m_{ij}(G)$ for all $(i,j) \in K$, and

   $$\widehat{\chi} = \left(1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{2}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{8}}, \frac{1}{3}, \frac{1}{\sqrt{12}}, \frac{1}{4}\right)^\top \in \mathbb{R}^9.$$

2. *Now consider the harmonic index $\mathcal{H} = \left(\frac{2}{i+j}\right) \in \mathbb{R}^{10}$. The partition on K induced by $\mathcal{H}$ is*

   $$[1,1] < [1,2] < [1,3] < [1,4] < [2,4] < [3,4] < [4,4]\,.$$

   Note that in this case $(2,2) \in [1,3]$, $(2,3) \in [1,4]$ and $(3,3) \in [2,4]$. Hence $p = 7$ and for $G \in \mathcal{G}_5$,

   $$\widehat{m}_\mathcal{H}(G) = (m_{11}, m_{12}, m_{13} + m_{22}, m_{14} + m_{23}, m_{24} + m_{33}, m_{34}, m_{44})^\top \in \mathbb{R}^7,$$

   where $m_{ij} = m_{ij}(G)$ for all $(i,j) \in K$, and

   $$\widehat{\mathcal{H}} = \left(1, \frac{2}{3}, \frac{1}{2}, \frac{2}{5}, \frac{1}{3}, \frac{2}{7}, \frac{1}{4}\right)^\top \in \mathbb{R}^7.$$

Proposition 2.5 *Let $\varphi \in \mathbb{R}^h$. If $G, G' \in \mathcal{G}_n$ then*

$$\widehat{m}_{\varphi}(G) = \widehat{m}_{\varphi}(G') \Longrightarrow \varphi(G) = \varphi(G').$$

Proof. Assume that $\varphi = (\varphi_{ij}) \in \mathbb{R}^h$ and $G \in \mathcal{G}_n$. Let

$$[i_1, j_1], [i_2, j_2], \ldots, [i_p, j_p]$$

be the distinct equivalence classes that form a partition on K as in (4). Consider the vectors $\widehat{\varphi}$ and $\widehat{m}_{\varphi}$ defined in (5) and (6), respectively. By (2)

$$\begin{aligned}\varphi(G) &= m(G) \cdot \varphi = \sum_{(i,j)\in K} m_{ij}(G)\,\varphi_{ij} \\ &= \sum_{k=1}^{p} \widehat{m}_{i_k j_k}(G)\,\varphi_{i_k j_k} = \widehat{m}_{\varphi}(G) \cdot \widehat{\varphi}.\end{aligned}$$

Hence

$$\varphi(G) = \widehat{m}_{\varphi}(G) \cdot \widehat{\varphi}, \tag{7}$$

where the dot product is on $\mathbb{R}^p$. It follows easily from (7) that if $G, G' \in \mathcal{G}_n$ then

$$\widehat{m}_{\varphi}(G) = \widehat{m}_{\varphi}(G') \Longrightarrow \varphi(G) = \varphi(G').$$

■

The following question arises naturally: which VDB topological indices $\varphi \in \mathbb{R}^h$ have the discrimination property with respect to the $\widehat{m}_{\varphi}$-structure relation on $\mathcal{G}_n$? Equivalently, for which VDB topological indices $\varphi \in \mathbb{R}^h$ is the condition

$$\varphi(G) = \varphi(G') \Longrightarrow \widehat{m}_{\varphi}(G) = \widehat{m}_{\varphi}(G')$$

satisfied for all $G, G' \in \mathcal{G}_n$?

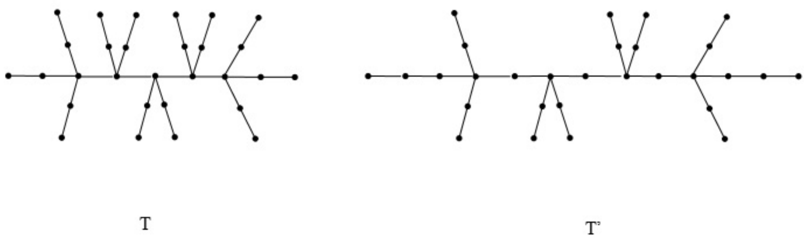

Figure 1. Trees with different $\widehat{m}_{\chi}$-structure but equal Randić index.

Example 2.6 *Consider the trees T and T' in $\mathcal{G}_{29}$ shown in Figure 1. Let χ be the Randić index. Note that all components of $\widehat{m}_{\chi}(T)$ are zero except*

$$\widehat{m}_{12}(T) = 12 \quad , \quad \widehat{m}_{24}(T) = 12 \quad , \quad \widehat{m}_{44}(T) = 4.$$

On the other hand, all components of $\widehat{m}_{\chi}(T')$ are zero except

$$\widehat{m}_{12}(T') = 10 \quad , \quad \widehat{m}_{14}(T') = 2 \quad , \quad \widehat{m}_{24}(T') = 16.$$

So clearly $\widehat{m}_{\chi}(T) \neq \widehat{m}_{\chi}(T')$. However, $\chi(T) = \chi(T') = \frac{36+2\sqrt{2}}{2\sqrt{2}}$. Hence, the Randić index does not have the discrimination property with respect to the $\widehat{m}_{\chi}$-relation on $\mathcal{G}_n$.

Most likely none of the VDB topological indices φ listed in Table 1 have the discrimination property with respect to the $\widehat{m}_{\varphi}$-relation on $\mathcal{G}_n$. However, we will show in the next section that we can define new VDB topological indices derived from those of the list in Table 1, that do have the discrimination property with respect to the $\widehat{m}_{\varphi}$-relation on $\mathcal{G}_n$.

3 Exponential VDB topological indices

We begin this section with the definition of exponential VDB topological indices.

Definition 3.1 *The exponential of $\varphi = (\varphi_{ij}) \in \mathbb{R}^h$ is the vector $\psi = e^{\varphi} \in \mathbb{R}^h$ defined as $\psi_{ij} = e^{\varphi_{ij}}$ for all $(i,j) \in K$.*

Example 3.2 *The exponential of the Randić index χ is $e^{\chi} = \left(e^{\frac{1}{\sqrt{ij}}}\right)_{(i,j)\in K}$.*

We will show in this section that the exponentials of the VDB topological indices φ in the list given in Table 1 have the discrimination property with respect to the $\widehat{m}_{\varphi}$-relation on $\mathcal{G}_n$. First we need to recall some facts about algebraic numbers.

An algebraic number is a complex number that is a root of a non-zero polynomial with rational coefficients. We will denote by $\mathcal{A}$ the field of algebraic numbers. Clearly $\mathbb{Q} \subseteq \mathcal{A}$, where $\mathbb{Q}$ is the set of rational numbers. Moreover, $\sqrt{q} \in \mathcal{A}$ for all $q \in \mathbb{Q}$, since $\sqrt{q}$ is a root of the polynomial $x^2 - q$.

Theorem 3.3 *[1] (Lindemann-Weierstrass's Theorem) If $\alpha_1, \ldots, \alpha_n$ are distinct algebraic numbers then, $e^{\alpha_1}, \ldots, e^{\alpha_n}$ are linearly independent over $\mathcal{A}$.*

Based on the classical theorem of Lindemann-Weierstrass we proof one of the main results of this paper.

Theorem 3.4 *Let $\varphi = (\varphi_{ij}) \in \mathbb{R}^h$ such that $\varphi_{ij} \in \mathcal{A}$ for all $(i,j) \in K$. Then e^φ has the discrimination property with respect to the $\widehat{m}_\varphi$-relation on $\mathcal{G}_n$.*

Proof. By Proposition 2.5, if $G, G' \in \mathcal{G}_n$ then

$$\widehat{m}_\varphi(G) = \widehat{m}_\varphi(G') \Longrightarrow e^\varphi(G) = e^\varphi(G').$$

Let

$$[i_1, j_1], [i_2, j_2], \ldots, [i_p, j_p]$$

be the distinct equivalence classes that form a partition on K induced by φ, as in (4). Consider the vectors $\widehat{\varphi}$ and $\widehat{m}_\varphi$ defined in (5) and (6), respectively. By (2)

$$\begin{aligned} e^\varphi(G) &= m(G) \cdot e^\varphi = \sum_{(i,j)\in K} m_{ij}(G)\, e^{\varphi_{ij}} \\ &= \sum_{k=1}^{p} \widehat{m}_{i_k j_k}(G)\, e^{\varphi_{i_k j_k}} = \widehat{m}_\varphi(G) \cdot e^{\widehat{\varphi}} \end{aligned} \tag{8}$$

Consequently, if $G, G' \in \mathcal{G}_n$ and $e^\varphi(G) = e^\varphi(G')$ then by (8)

$$0 = [\widehat{m}_\varphi(G) - \widehat{m}_\varphi(G')] \cdot e^{\widehat{\varphi}}$$

By hypothesis, $\varphi_{i_k j_k} \in \mathcal{A}$ for all $k = 1, \ldots, p$. Moreover, $\varphi_{i_1 j_1}, \ldots, \varphi_{i_p j_p}$ are distinct algebraic numbers since $[i_1, j_1], [i_2, j_2], \ldots, [i_p, j_p]$ are distinct equivalence classes. On the other hand, since all components of $\widehat{m}_\varphi(G) - \widehat{m}_\varphi(G')$ are integers, it follows from Theorem 3.3 that $\widehat{m}_\varphi(G) = \widehat{m}_\varphi(G')$. ■

Corollary 3.5 *The exponential of all VDB topological indices φ in the list given in Table 1 have the discrimination property with respect to the $\widehat{m}_\varphi$-relation on $\mathcal{G}_n$.*

Proof. It is easy to see that for all $\varphi = (\varphi_{ij})$ in the list given in Table 1, $\varphi_{ij} \in \mathcal{A}$ for all $(i,j) \in K$. The result follows from Theorem 3.4. ■

Example 3.6 *As we noted in Example 2.6, the Randić index χ does not discriminate between the trees T and T' of Figure 1, which have different $\widehat{m}_\chi$-structure. However, $e^\chi(T) \neq e^\chi(T')$. In fact,*

$$e^\chi(T) = 12e^{\frac{1}{\sqrt{2}}} + 12e^{\frac{1}{\sqrt{8}}} + 4e^{\frac{1}{4}} \approx 46.56$$

and

$$e^\chi(T') = 10e^{\frac{1}{\sqrt{2}}} + 2e^{\frac{1}{2}} + 16e^{\frac{1}{\sqrt{8}}} \approx 46.36.$$

4 Extremal values of Randić's exponential index over $\mathcal{G}_n$

In view of the nice mathematical properties exponential VDB topological indices have, given $\varphi = (\varphi_{ij}) \in \mathbb{R}^h$ such that $\varphi_{ij} \in \mathcal{A}$ for all $(i,j) \in K$, an interesting problem is to find the extremal values of e^{φ} over $\mathcal{G}_n$. Note that if $\varphi \in \mathbb{R}^h$ and $G \in \mathcal{G}_n$, in general $e^{\varphi}(G) \neq e^{\varphi(G)}$. For instance, if S_n is the star tree with n vertices and χ the Randić index, then $\chi(S_n) = \sqrt{n-1}$ and $e^{\chi}(S_n) = (n-1)\, e^{\frac{1}{\sqrt{n-1}}}$. Consequently, it is not possible to deduce the extremal values of e^{φ} directly from the extremal values of φ over $\mathcal{G}_n$.

In our next results we find the extremal value of Randić's exponential index over $\mathcal{G}_n$. Let us recall some results from [22]. The support of a graph $G \in \mathcal{G}_n$ is denoted by $Supp(G)$ and defined as

$$Supp(G) = \{(p,q) \in K : m_{pq}(G) > 0\}.$$

We define the reference vector $\mathcal{R} = (\mathcal{R}_{pq}) \in \mathbb{R}^h$ as the vector with coordinates $\mathcal{R}_{pq} = \frac{p+q}{pq}$, for all $(p,q) \in K$.

Corollary 4.1 *[22, Corollaries 3.8 and 3.13] Let $G_0 \in \mathcal{G}_n$ and assume that $Supp(G_0) = \{(p_0,q_0)\}$.*

1. *If $\varphi \in \mathbb{R}^h$ satisfies $\varphi \geq k_0\mathcal{R}$, where $k_0 = \frac{p_0q_0}{p_0+q_0}\varphi_{p_0q_0}$, then G_0 attains the minimum value of φ over $\mathcal{G}_n$;*
2. *If $\psi \in \mathbb{R}^h$ satisfies $\psi \leq k_0\mathcal{R}$, where $k_0 = \frac{p_0q_0}{p_0+q_0}\psi_{p_0q_0}$, then G_0 attains the maximum value of ψ over $\mathcal{G}_n$.*

Based on this result we next find the extremal values of Randić's exponential index e^{χ} over $\mathcal{G}_n$. First a technical lemma.

Lemma 4.2 *Let n be an integer, $n \geq 2$. The function $f(x) = \frac{xne^{\frac{1}{\sqrt{xn}}}}{x+n}$ is increasing in the interval $[1,n]$.*

Proof. The derivative is

$$f'(x) = \frac{1}{2}n^2xe^{\frac{1}{\sqrt{nx}}}\frac{2n\sqrt{nx}-n-x}{\left(\sqrt{nx}\right)^3(n+x)^2}$$

Note that when $1 \le x \le n$ then

$$\begin{aligned} 2n\sqrt{nx} - n - x &\ge 2n\sqrt{x^2} - n - x \\ &= (2n-1)\,x - n \\ &\ge (2n-1) - n = n - 1 \ge 0 \end{aligned}$$

Hence f is increasing in the interval $[1, n]$. ■

Theorem 4.3 *Let $n \ge 2$ and χ the Randić index. Among all graphs in $\mathcal{G}_n$:*

1. *The minimal value of e^{χ} is attained in the star S_n;*
2. *The maximal value of e^{χ} is attained in the complete graph K_n.*

Proof. 1. Clearly $Supp\,(S_n) = \{(1, n-1)\}$. Let $k_0 = \frac{n-1}{n}e^{\frac{1}{\sqrt{n-1}}}$. We will show that

$$e^{\frac{1}{\sqrt{ij}}} \ge \frac{n-1}{n}e^{\frac{1}{\sqrt{n-1}}}\frac{i+j}{ij}$$

for all $(i, j) \in K$. Equivalently,

$$\frac{ije^{\frac{1}{\sqrt{ij}}}}{i+j} \ge \frac{n-1}{n}e^{\frac{1}{\sqrt{n-1}}} \tag{9}$$

for all $(i, j) \in K = \{(i, j) \in \mathbb{N} \times \mathbb{N} : 1 \le i \le j \le n-1\}$.

We proceed by induction on n. If $n = 2$ then $K = \{(1, 1)\}$ and equality occurs in (9). Assume that (9) holds for all $(i, j) \in K$. Let $\widehat{K} = \{(i, j) \in \mathbb{N} \times \mathbb{N} : 1 \le i \le j \le n\}$. By our induction hypothesis and the fact that

$$\left\{\frac{n-1}{n}e^{\frac{1}{\sqrt{n-1}}}\right\}_{n\ge 2}$$

is a decreasing sequence (elementary calculus), for all $(i, j) \in \widehat{K}$ such that $1 \le i \le j \le n-1$

$$\frac{ije^{\frac{1}{\sqrt{ij}}}}{i+j} \ge \frac{n-1}{n}e^{\frac{1}{\sqrt{n-1}}} \ge \frac{n}{n+1}e^{\frac{1}{\sqrt{n}}}.$$

The remaining case is when $j = n$ and $1 \le i \le n$. By Lemma 4.2,

$$\frac{ine^{\frac{1}{\sqrt{in}}}}{i+n} = f\,(i) \ge f\,(1) = \frac{n}{n+1}e^{\frac{1}{\sqrt{n}}}$$

for all $1 \le i \le n$. We have shown that

$$\frac{ije^{\frac{1}{\sqrt{ij}}}}{i+j} \ge \frac{n}{n+1}e^{\frac{1}{\sqrt{n}}},$$

for all $(i,j) \in \widehat{K}$, so the induction is complete. It follows from part 1 of Corollary 4.1, that the minimal value of e^{χ} is attained in the star S_n.

2. The support of K_n is $Supp\,(K_n) = \{(n-1, n-1)\}$. Let $k_0 = \frac{n-1}{2}e^{\frac{1}{n-1}}$. We will show that

$$\frac{ije^{\frac{1}{\sqrt{ij}}}}{i+j} \leq \frac{n-1}{2}e^{\frac{1}{n-1}}, \tag{10}$$

for all $(i,j) \in K$. Again we proceed by induction. If $n = 2$ then $K = \{(1,1)\}$ and equality occurs in (10). Assume that (10) holds for all $(i,j) \in K$. Let $\widehat{K} = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leq i \leq j \leq n\}$. By the induction hypothesis and the fact that

$$\left\{\frac{n-1}{2}e^{\frac{1}{n-1}}\right\}_{n \geq 2}$$

is an increasing sequence (elementary calculus), we deduce

$$\frac{ije^{\frac{1}{\sqrt{ij}}}}{i+j} \leq \frac{n-1}{2}e^{\frac{1}{n-1}} \leq \frac{n}{2}e^{\frac{1}{n}},$$

for all $(i,j) \in \widehat{K}$ such that $1 \leq i \leq j \leq n-1$. When $j = n$ and $1 \leq i \leq n$, we deduce

$$\frac{ine^{\frac{1}{\sqrt{in}}}}{i+n} = f\,(i) \leq f\,(n) = \frac{n}{2}e^{\frac{1}{n}},$$

by Lemma 4.2. So the induction is complete. It follows from part 2 of Corollary 4.1, that the maximal value of e^{χ} is attained in the complete graph K_n. ■

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