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Is Every Graph the Extremal Value of a Vertex–Degree–Based Topological Index?

Juan Rada[1] , Sergio Bermudo[2]

[1]*Instituto de Matemáticas, Universidad de Antioquia*
Medellín, Colombia

[2]*Department of Economy, Quantitative Methods and Economic History,*
Pablo de Olavide University. Carretera de Utrera Km. 1,
41013-Sevilla, Spain

pablo.rada@udea.edu.co, sbernav@upo.es

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Abstract

Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. In this paper we identify vertex–degree–based topological indices over $\mathcal{G}_n$ with vectors in $\mathbb{R}^h$, the Euclidean space with $h = \frac{(n-1)n}{2}$ coordinates. In this setting, we give an interpretation of the extremal values of a topological index in terms of angles between vectors in $\mathbb{R}^h$. Then we consider the following problem: given a graph $G_0 \in \mathcal{G}_n$, does there exist a vertex–degree–based topological index that attains its extremal values in G_0? The answer is affirmative. In order to do this, we introduce the support of the graph G_0, the reference vector, and then construct vectors such that G_0 is an extremal value.

1 Introduction

In the chemical literature, a great variety of topological indices (molecular structure descriptors) have been and are currently considered in applications to QSPR/QSAR studies [1, 11, 12]. Many of them depend only on the degrees of the vertices of the underlying molecular graph and are now called vertex–degree–based topological indices. More precisely, given nonnegative numbers $\{\varphi_{ij}\}$, a vertex–degree–based topological index is expressed as

$$TI = TI(G) = \sum_{1 \le i \le j \le n-1} m_{ij}\varphi_{ij} \tag{1}$$

where G is a (molecular) graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. For instance, $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ pertains to the Randić connectivity index [10], one of the classical vertex–degree–based topological indices with more applications in chemistry and pharmacology. Details on this and others degree–based–topological indices can be found in [2–8] and the references cited therein.

Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. In Section 2 of this paper we give a one-to-one correspondence between vertex–degree–based topological indices over $\mathcal{G}_n$ and vectors in $\mathbb{R}^h$, the Euclidean space with $h = \frac{(n-1)n}{2}$ coordinates. So we can identify vertex–degree–based topological indices with vectors. In this setting, we give an interpretation of the extremal values of a topological index in terms of angles between vectors in $\mathbb{R}^h$.

One important problem that appears frequently in the mathematical-chemistry literature is to find the extremal values of well known topological indices over the class of graphs with equal number of vertices. In Section 3 we consider the inverse problem: given a graph $G_0 \in \mathcal{G}_n$, does there exist a vertex–degree–based topological index that attains its extremal values in G_0? The answer is affirmative. In order to do this, we introduce the support of the graph G_0, the reference vector, and then construct vectors in Theorems 3.5 and 3.10 such that G_0 is an extremal value.

The proof of our main result strongly relies on [9, Theorem 2.3]. Let TI be a vertex–degree–based topological index defined from the numbers $\{\varphi_{ij}\}$ as in (1). Consider the numbers $f_{ij} = \frac{ij\varphi_{ij}}{i+j}$, where (i, j) belongs to the set

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

Define the sets

$$K_{\min}(f) = \left\{(r,s) \in K : \ f_{rs} = \min_{(i,j)\in K} f_{ij}\right\}$$

and

$$K_{\max}(f) = \left\{(p,q) \in K : \ f_{pq} = \max_{(i,j)\in K} f_{ij}\right\}.$$

The complements of $K_{\min}(f)$ and $K_{\max}(f)$ in K are denoted by $K^c_{\min}(f)$ and $K^c_{\max}(f)$, respectively.

Theorem 1.1 *[9] Let TI be a vertex–degree–based topological index as in (1) and define $f_{ij} = \frac{ij\varphi_{ij}}{i+j}$ for every $(i,j) \in K$. For every graph $G \in \mathcal{G}_n$*

$$n\left(\min_{(i,j)\in K} f_{ij}\right) \le TI\left(G\right) \le n\left(\max_{(i,j)\in K} f_{ij}\right).$$

Moreover, equality on the left occurs if and only if $m_{pq} = 0$ for all $(p,q) \in K^c_{min}(f)$. Equality on the right occurs if and only if $m_{rs} = 0$ for all $(r,s) \in K^c_{max}(f)$.

2 Geometric representation of vertex–degree–based topological indices

Let n be a positive integer. Consider the set

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

Note that K has exactly $h = \frac{(n-1)n}{2}$ elements. We order lexicographically the elements of K:

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

so we can express every vector of $\mathbb{R}^h$ as (φ_{ij}), where $\varphi_{ij} \in \mathbb{R}$ for all $(i,j) \in K$.

Recall that the dot product of two vectors $X = (x_{ij})_{(i,j)\in K}$ and $Y = (y_{ij})_{(i,j)\in K}$ of $\mathbb{R}^h$ is

$$X \cdot Y = \sum_{(i,j)\in K} x_{ij} y_{ij}.$$

Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. Consider the function $m : \mathcal{G}_n \longrightarrow \mathbb{R}^h$ defined by $m(G) = (m_{ij}(G))_{(i,j)\in K}$, where $G \in \mathcal{G}_n$. We next formally define a vertex–degree–based topological index over $\mathcal{G}_n$.

Definition 2.1 *A vertex–degree–based topological index is a function $T_\varphi : \mathcal{G}_n \longrightarrow \mathbb{R}$ defined as*

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

for all $G \in \mathcal{G}_n$, where $\varphi \in \mathbb{R}^h$.

So every vertex–degree–based topological index is of the form T_φ for some vector $\varphi \in \mathbb{R}^h$, and conversely, every vector $\varphi \in \mathbb{R}^h$ induces a vertex degree based topological index T_φ as in (2). In other words, vertex–degree–based topological indices can be identified with vectors in $\mathbb{R}^h$. From now on, if $G \in \mathcal{G}_n$ we write $\varphi(G)$ instead of $T_\varphi(G)$. In other words, if $G \in \mathcal{G}_n$ then

$$\varphi(G) = m(G) \cdot \varphi.$$

Example 2.2 *The Randić index over $\mathcal{G}_n$ is the vector $\varphi = \left(\frac{1}{\sqrt{ij}}\right)_{(i,j)\in K} \in \mathbb{R}^h$.*

Recall that the length of $X \in \mathbb{R}^h$ is $\|X\| = (X \cdot X)^{\frac{1}{2}}$. The angle between the two vectors X and Y of $\mathbb{R}^h$ is defined as the angle θ between 0 and π such that

$$\cos\theta = \frac{X \cdot Y}{\|X\| \, \|Y\|}. \tag{3}$$

The vectors are perpendicular if $\theta = \frac{\pi}{2}$. If $\theta < \frac{\pi}{2}$ (resp. $\theta > \frac{\pi}{2}$) then the angle is acute (resp. obtuse). It follows from (3) that the angle between X and Y is acute (resp. obtuse) if and only if $X \cdot Y > 0$ (resp. $X \cdot Y < 0$). If $X \cdot Y = 0$ then X and Y are perpendicular. We next give a geometric interpretation of the extremal values of a vertex–degree–based topological index over $\mathcal{G}_n$.

Theorem 2.3 *Let $G_0 \in \mathcal{G}_n$. G_0 attains the minimum value of the vertex–degree–based topological index $\varphi \in \mathbb{R}^h$ over $\mathcal{G}_n$ if and only if φ is perpedicular or forms an acute angle with $m(G) - m(G_0)$, for all $G \in \mathcal{G}_n$.*

Proof. Note that for all $G \in \mathcal{G}_n$

$$[m(G) - m(G_0)] \cdot \varphi = \varphi(G) - \varphi(G_0). \tag{4}$$

The result follows from (4) using the fact that G_0 attains the minimum value of φ if and only if $\varphi(G) - \varphi(G_0) \geq 0$. ∎

Similarly we have the following result.

Theorem 2.4 *Let $G_0 \in \mathcal{G}_n$. G_0 attains the maximum value of the vertex–degree–based topological index $\varphi \in \mathbb{R}^h$ over $\mathcal{G}_n$ if and only if φ is perpedicular or forms an obtuse angle with $m(G) - m(G_0)$, for all $G \in \mathcal{G}_n$.*

3 Is every graph the extremal value of a vertex degree based topological index?

One fundamental problem in chemical graph theory is to determine the extremal values of a given vertex–degree–based topological index over $\mathcal{G}_n$. Now we consider the inverse problem: given a graph $G_0 \in \mathcal{G}_n$, does there exist $\varphi \in \mathbb{R}^h$ such that G_0 is an extremal value of φ over $\mathcal{G}_n$?

Definition 3.1 *The support of a graph $G \in \mathcal{G}_n$ is denoted by $Supp\,(G)$ and defined as*

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

Example 3.2 *We compute the support of several graphs:*

1. *If S_n is the star tree with n vertices then $Supp\,(S_n) = \{(1, n-1)\}$;*
2. *If K_n is the complete graph with n vertices then $Supp\,(K_n) = \{(n-1, n-1)\}$;*
3. *If P_n is the path tree with n vertices then $Supp\,(P_n) = \{(1,2)\,, (2,2)\}$.*

Definition 3.3 *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 $(p,q) \in K$.*

Example 3.4 *If $n = 4$ then $h = \frac{4 \cdot 3}{2} = 6$ and the reference vector $\mathcal{R} = (\mathcal{R}_{pq}) \in \mathbb{R}^6$ is*

$$\mathcal{R} = \begin{pmatrix} 2 & 3/2 & 4/3 \\ * & 1 & 5/6 \\ * & * & 2/3 \end{pmatrix}.$$

Let $X = (x_{ij})_{(i,j)\in K}$ and $Y = (y_{ij})_{(i,j)\in K}$ be two vectors of $\mathbb{R}^h$. We write $X \geq Y$ to indicate that $x_{ij} \geq y_{ij}$ for all $(i,j) \in K$. Also, if $L \subseteq K$ then $X\,|_{L} = Y\,|_{L}$ means $x_{ij} = y_{ij}$ for all $(i,j) \in L$.

Now we can state and prove our main result. We denote by $Supp^c\,(G)$ the complement of $Supp\,(G)$ in K.

Theorem 3.5 *Let $G_0 \in \mathcal{G}_n$ and k a positive number. If $\varphi \in \mathbb{R}^h$ is such that $\varphi \geq k\mathcal{R}$ and $\varphi\Big|_{Supp(G_0)} = k\mathcal{R}\Big|_{Supp(G_0)}$, then φ attains its minimum value over $\mathcal{G}_n$ in G_0 and $\varphi\,(G_0) = nk$.*

Proof. Consider the vector $\varphi = (\varphi_{pq}) \in \mathbb{R}^h$ such that $\varphi \geq k\mathcal{R}$ and $\varphi\Big|_{Supp(G_0)} = k\mathcal{R}\Big|_{Supp(G_0)}$. Let $f_{pq} = \frac{pq\varphi_{pq}}{p+q}$, for every $(p,q) \in K$. Clearly, $f_{pq} = k$ for every $(p,q) \in Supp\,(G_0)$ and $f_{pq} \geq k$ for every $(p,q) \in Supp^c\,(G_0)$. Consequently, $k = \min_{(i,j)\in K} f_{ij}$ and $Supp\,(G_0) \subseteq K_{\min}(f)$. Then $K^c_{\min}(f) \subseteq Supp^c\,(G_0)$ which implies $m_{ij}(G_0) = 0$ for all $(i,j) \in K^c_{\min}(f)$. Hence by Theorem 1.1

$$\varphi(G) \geq n \min_{(i,j)\in K} f_{ij} = nk = \varphi(G_0),$$

for every graph $G \in \mathcal{G}_n$. Consequently, φ attains its minimum value in G_0 over $\mathcal{G}_n$ and $\varphi(G_0) = nk$. ■

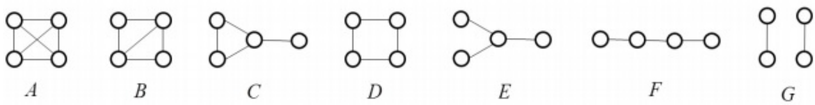

Figure 1. Graphs in $\mathcal{G}_4$

Corollary 3.6 *Let $G_0 \in \mathcal{G}_n$ and l_0 a positive number. There exists a topological index $\varphi \in \mathbb{R}^h$ that attains its minimum value in G_0 over $\mathcal{G}_n$ and $\varphi(G_0) = l_0$.*

Proof. Choose $\varphi = (\varphi_{pq}) \in \mathbb{R}^h$ such that $\varphi \geq \frac{l_0}{n}\mathcal{R}$ and $\varphi\Big|_{Supp(G_0)} = \frac{l_0}{n}\mathcal{R}\Big|_{Supp(G_0)}$. Then by Theorem 3.5, $\varphi \in \mathbb{R}^h$ attains its minimal value in G_0 over $\mathcal{G}_n$ and $\varphi(G_0) = n\frac{l_0}{n} = l_0$. ■

Example 3.7 *Consider the following problem: among all graphs in $\mathcal{G}_4$ (see Figure 1), find a vertex–degree–based topological index φ such that C has minimum value over $\mathcal{G}_4$ and $\varphi(C) = 2$. As in the proof of Corollary 3.6, we compute the vector $\frac{l_0}{n}\mathcal{R}$, which in this case is*

$$\frac{1}{2}\mathcal{R} = \frac{1}{2}\begin{pmatrix} 2 & 3/2 & 4/3 \\ * & 1 & 5/6 \\ * & * & 2/3 \end{pmatrix}.$$

Note that $Supp\,(C) = \{(1,3),(2,2),(2,3)\}$. Choose a vector $\varphi \geq \frac{1}{2}\mathcal{R}$ such that

$$\varphi\Big|_{\{(1,3),(2,2),(2,3)\}} = \frac{1}{2}\mathcal{R}\Big|_{\{(1,3),(2,2),(2,3)\}}.$$

For instance,

$$\varphi = \frac{1}{2}\begin{pmatrix} 2 & 2 & 4/3 \\ * & 1 & 5/6 \\ * & * & 1 \end{pmatrix}.$$

Then by Theorem 3.5, φ attains its minimum value in C over $\mathcal{G}_4$ and $\varphi(C) = 2$. In fact,

$$\begin{array}{lcl} \varphi(A) = 6(1/2) = 3 & ; & \varphi(E) = 3(2/3) = 2 \\ \varphi(B) = 4(5/12) + 1/2 = 13/6 & ; & \varphi(F) = 2(1) + 1/2 = 5/2 \\ \varphi(C) = 1/2 + 2/3 + 2(5/12) = 2 & ; & \varphi(G) = 2(1) = 2. \\ \varphi(D) = 4(1/2) = 2 & ; & \end{array}$$

It is well known that the star tree S_n and the complete graph K_n are extremal values of many important vertex–degree–based topological indices over $\mathcal{G}_n$. Theorem 3.5 can explain this, as we shall see in our next results. Note that $Supp(S_n) = \{(1, n-1)\}$ and $Supp(K_n) = \{(n-1, n-1)\}$. In both cases, the support has exactly one element.

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

Proof. Since $\varphi \geq k_0\mathcal{R}$ and the coordinate p_0q_0 of $k_0\mathcal{R}$ is

$$k_0 \frac{p_0 + q_0}{p_0q_0} = \left(\frac{p_0q_0}{p_0 + q_0}\varphi_{p_0q_0}\right)\frac{p_0 + q_0}{p_0q_0} = \varphi_{p_0q_0},$$

we deduce the result from Theorem 3.5. ■

Example 3.9 *Let S_n be the star tree with n vertices. Note that $Supp(S_n) = \{(1, n-1)\}$. By Corollary 3.8, S_n is the minimum value of any vertex–degree–based topological index $\varphi = (\varphi_{pq}) \in \mathbb{R}^h$ over $\mathcal{G}_n$ that satisfies*

$$\varphi_{pq} \geq \frac{p+q}{pq}\frac{n-1}{n}\varphi_{1,n-1} \tag{5}$$

for all $(p, q) \in K$. Note that for the Randić index $\varphi_{pq} = \frac{1}{\sqrt{pq}}$, geometric-arithmetic index $\varphi_{pq} = \frac{2\sqrt{pq}}{p+q}$, harmonic index $\varphi_{pq} = \frac{2}{p+q}$, sum-connectivity index $\frac{1}{\sqrt{p+q}}$ and augmented Zagreb index $\varphi_{pq} = \left(\frac{pq}{p+q-2}\right)^3$, condition (5) holds. Hence, for each of these indices, the star attains its minimum value over $\mathcal{G}_n$.

Similarly, we have the dual results of Theorem 3.5, Corollaries 3.6 and 3.8.

Theorem 3.10 *Let $G_0 \in \mathcal{G}_n$ and k a positive number. If $\psi \in \mathbb{R}^h$ is such that $\psi \leq k\mathcal{R}$ and $\psi\Big|_{Supp(G_0)} = k\mathcal{R}\Big|_{Supp(G_0)}$, then ψ attains its maximum value over $\mathcal{G}_n$ in G_0 and $\psi(G_0) = nk$.*

Corollary 3.11 *Let $G_0 \in \mathcal{G}_n$ and m_0 a positive number. There exists a topological index $\psi \in \mathbb{R}^h$ that attains its maximum value in G_0 over $\mathcal{G}_n$ and $\psi(G_0) = m_0$.*

Example 3.12 *Let us find a topological index ψ over $\mathcal{G}_4$ such that F has maximum value and $\psi(F)=1$ (see Figure 1). The support of F is $\{(1,2),(2,2)\}$. So we choose a vector $\psi \leq \frac{1}{4}\mathcal{R}$ such that $\psi\Big|_{\{(1,2),(2,2)\}} = \frac{1}{4}\mathcal{R}\Big|_{\{(1,2),(2,2)\}}$. For example,*

$$\psi = \frac{1}{4}\begin{pmatrix} 3/2 & 3/2 & 1 \\ * & 1 & 2/3 \\ * & * & 1/3 \end{pmatrix} \leq \frac{1}{4}\begin{pmatrix} 2 & 3/2 & 4/3 \\ * & 1 & 5/6 \\ * & * & 2/3 \end{pmatrix} = \frac{1}{4}\mathcal{R}.$$

Hence, by Theorem 3.10, ψ attains its maximum value in F over $\mathcal{G}_4$ and $\psi(F)=1$. In fact,

$$\begin{array}{lcl} \psi(A) = 6(1/12) = 1/2 & ; & \psi(E) = 3(1/4) = 3/4 \\ \psi(B) = 4(1/6) + 1/12 = 3/4 & ; & \psi(F) = 2(3/8) + 1/4 = 1 \\ \psi(C) = 1/4 + 1/4 + 2(1/6) = 5/6 & ; & \psi(G) = 2(3/8) = 3/4. \\ \psi(D) = 4(1/4) = 1 & & \end{array}$$

Corollary 3.13 *Let $G_0 \in \mathcal{G}_n$ and assume that $Supp(G_0) = \{(p_0, q_0)\}$. If $\psi \in \mathbb{R}^h$ satisfies $\psi \leq k_0\mathcal{R}$, where $k_0 = \frac{p_0 q_0}{p_0+q_0}\psi_{p_0q_0}$, then G_0 attains the maximum value of ψ over $\mathcal{G}_n$.*

Example 3.14 *Let K_n be the complete graph with n vertices. Then*

$$Supp(K_n) = \{(n-1, n-1)\}.$$

By Corollary 3.13, K_n is the maximum value of any vertex–degree–based topological index $\psi = (\psi_{ij}) \in \mathbb{R}^h$ over $\mathcal{G}_n$ that satisfies

$$\psi_{pq} \leq \frac{p+q}{pq}\frac{n-1}{2}\psi_{n-1,n-1} \tag{6}$$

for all $(p,q) \in K$. For instance, the first Zagreb index $\psi_{pq} = p+q$, the second Zagreb index $\psi_{pq} = pq$, the Randić index $\psi_{pq} = \frac{1}{\sqrt{pq}}$, the harmonic index $\psi_{pq} = \frac{2}{p+q}$, the geometric-arithmetic index $\psi_{pq} = \frac{2\sqrt{pq}}{p+q}$, the sum-connectivity index $\psi_{pq} = \frac{1}{\sqrt{p+q}}$, the ABC index $\psi_{pq} = \sqrt{\frac{p+q-2}{pq}}$ and the augmented Zagreb $\psi_{pq} = \left(\frac{pq}{p+q-2}\right)^3$ satisfy condition (6). Hence, for each of these indices, the complete graph K_n attains its maximum value over $\mathcal{G}_n$.

Corollary 3.15 *Let G_0 and G_1 be two graphs such that $Supp(G_0) \cap Supp(G_1) = \emptyset$, and let $l_0 < l_1$ be two positive numbers. There exists a topological index φ which attains its minimum and maximum value over $\mathcal{G}_n$ in G_0 and G_1, respectively, and $\varphi(G_0) = l_0$ and $\varphi(G_1) = l_1$.*

Proof. Define $\varphi = (\varphi_{pq}) \in \mathbb{R}^h$ such that $\frac{l_0}{n}\mathcal{R} \leq \varphi \leq \frac{l_1}{n}\mathcal{R}$, $\varphi\Big|_{Supp(G_0)} = \frac{l_0}{n}\mathcal{R}\Big|_{Supp(G_0)}$ and $\varphi\Big|_{Supp(G_1)} = \frac{l_1}{n}\mathcal{R}\Big|_{Supp(G_1)}$. Then proceed as in Theorems 3.5 and 3.10. ■

One final comment. The most important vertex–degree–based topological indices are vectors which derive from symmetric functions (for instance, the Randić index $\frac{1}{\sqrt{pq}}$, the geometric-arithmetic index $\frac{2\sqrt{pq}}{p+q}$, etc ....). What about the vectors that are not of this type, are they interesting in applications to QSPR/QSAR?

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