Extremal (n,m)-graphs with respect to VDB topological indices

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Abstract: The vertex-degree based (VDB) topological index (or graphical function-index) $TI_f(G)$ of G with edge-weight function $f(x,y)$ was defined as $TI_f(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where $d(u)$ is the degree of vertex u in G. In this paper, we use a unified way to determine the extremal values of VDB indices of connected (n,m)-graphs. When $f(x,y)$ satisfies some special properties, we determine the connected (n,m)-graphs with maximum (or minimum) $TI_f(G)$ is the almost regular graphs. Our results generalize the results of paper [Aashtab, A., Akbari, S., Madadinia, S., Noei, M., & Salehi, F. (2022) On the graphs with minimum Sombor index. MATCH Commun. Math. Comput. Chem., 88, 553-559].

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. $|V(G)| = n$ is the number of vertices, $|E(G)| = m$ is the number of edges of G. The set of graphs with $|V(G)| = n$ and $|E(G)| = m$ are called (n,m) graphs. Denote by $N_G(u)$ the set of vertices which are neighbors of the vertex u. Then $|N_G(u)|$ is the degree of vertex u, denoted by d_u. Let $\Delta(G)$, $\delta(G)$ be the maximum degree, minimum degree of G. For all notations and terminology used, but not defined here, we refer to the textbook [1].

Let $f(x,y)$ be a symmetric real function, $d(u)$ the degree of vertex u in G. The vertex-degree based topological (or graphical function-index) $TI_f(G)$ of G with edge-weight function $f(x,y)$ was defined as [2]

$$TI_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)). \tag{1}$$

There are several research on extremal VDB topological indices, see [3–10]. Gutman [11] listed most of the VDB indices, we show in the Table 1.

If $f(x,y)$ is monotonically increasing on x (or y), $h(x) = f(a,x) - f(b,x)$ is monotonically decreasing on x for any $a \ge b \ge 0$, then we call $f(x,y)$ is the first good function.

If $f(x,y)$ is monotonically decreasing on x (or y), $h(x) = f(a,x) - f(b,x)$ is monotonically increasing on x for any $a \ge b \ge 0$, then we call $f(x,y)$ is the second good function.

The present paper was motivated by a recent paper of Aashtab *et al.*, [12] on Sombor index, where they study the structure of a graph with minimum Sombor index among all graphs with fixed order and fixed size. They shown that in every graph with minimum Sombor index the difference between minimum and maximum degrees is at most 1. We take further the line of considering the extremal values of VDB topological indices of connected (n,m)-graphs by a unified way. We obtain some properties of extremal connected (n,m)-graphs with respect to VDB topological indices.

Table 1. VDB topological indices

Function $f(x,y)$	Equation (1) corresponds to	Symbol
$1/\sqrt{xy}$	Randić index [13]	R
$\sqrt{x^2+y^2}$	Sombor index [11]	SO
$\sqrt{x+y-2/xy}$	atom-bond connectivity index [14]	ABC
$x+y$	first Zagreb index [15,16]	M_1
xy	second Zagreb index [17]	M_2
$1/\sqrt{x+y}$	sum-connectivity index [18]	χ
$[xy/(x+y-2)]^3$	augmented Zagreb index [19]	AZI
$\sqrt{xy}$	reciprocal Randić index [20]	RR
x^2+y^2	forgotten topological index [15]	F
$2xy/(x+y)$	inverse sum indeg index [21]	ISI
$2/(x+y)$	harmonic index [22]	H
$2\sqrt{xy}/(x+y)$	geometric-arithmetic index [23]	GA
$(x+y)/(2\sqrt{xy})$	arithmetic-geometric index [24]	AG
$1/x^2+1/y^2$	inverse degree index [22]	ID
$|x-y|$	Albertson index [25]	Alb
$y/x+x/y$	symmetric division deg index [21]	SDD

2. Main Results

Theorem 1. *Let G be a connected (n,m) graph and $f(x,y)$ is the first good function. For any $a > b+1 \geq 2$, $H(a,b) > 0$, where $H(a,b) = a[f(a,a) - f(a-1,a)] - b[f(b+1,b) - f(b,b)]$. If $TI_f(G)$ has the minimum value in G, then G is an almost regular graph, i.e., $\Delta(G) - \delta(G) \leq 1$.*

Proof. On the contrary, we suppose G is not an almost regular graph, i.e., $\Delta(G) - \delta(G) \geq 2$. Let $d(u) = \Delta$, $d(v) = \delta$.

Case 1. $uv \notin E(G)$.

Let $N_G(u) = \{u_1, u_2, \cdots, u_\Delta\}$, $N_G(v) = \{v_1, v_2, \cdots, v_\delta\}$. Since $\Delta(G) - \delta(G) \geq 2$, we suppose $u_\Delta \notin N_G(v)$. Let $S \subseteq E(G)$ be the set of edges which adjacent to u or v. Let $G^* = G - uu_\Delta + vu_\Delta$.

$$TI_f(G) = \sum_{uv \in E(G) \smallsetminus S} f(d(u), d(v)) + \sum_{i=1}^{\Delta} f(\Delta, d(u_i)) + \sum_{i=1}^{\delta} f(\delta, d(v_i)).$$

$$TI_f(G^*) = \sum_{uv \in E(G) \smallsetminus S} f(d(u), d(v)) + \sum_{i=1}^{\Delta-1} f(\Delta-1, d(u_i)) + \sum_{i=1}^{\delta} f(\delta+1, d(v_i)) + f(d(u_\Delta), \delta+1).$$

$$
\begin{aligned}
TI_f(G) - TI_f(G^*) &= \sum_{i=1}^{\Delta-1}[f(\Delta, d(u_i)) - f(\Delta-1, d(u_i))] - \sum_{i=1}^{\delta}[f(\delta+1, d(v_i)) - f(\delta, d(v_i))] \\
&\quad + f(\Delta, d(u_\Delta)) - f(\delta+1, d(u_\Delta)) \\
&= \sum_{i=1}^{\Delta}[f(\Delta, d(u_i)) - f(\Delta-1, d(u_i))] - \sum_{i=1}^{\delta}[f(\delta+1, d(v_i)) - f(\delta, d(v_i))] \\
&\quad + f(\Delta-1, d(u_\Delta)) - f(\delta+1, d(u_\Delta)) \\
&\geq \sum_{i=1}^{\Delta}[f(\Delta, d(u_i)) - f(\Delta-1, d(u_i))] - \sum_{i=1}^{\delta}[f(\delta+1, d(v_i)) - f(\delta, d(v_i))] \\
&\geq \sum_{i=1}^{\Delta}[f(\Delta, \Delta) - f(\Delta-1, \Delta)] - \sum_{i=1}^{\delta}[f(\delta+1, \delta) - f(\delta, \delta)] \\
&= \Delta[f(\Delta, \Delta) - f(\Delta-1, \Delta)] - \delta[f(\delta+1, \delta) - f(\delta, \delta)] > 0.
\end{aligned}
$$

Case 2. $uv \in E(G)$.

Let $N_G(u) = \{u_1, u_2, \cdots, u_{\Delta-1}, v\}$, $N_G(v) = \{v_1, v_2, \cdots, v_{\delta-1}, u\}$. Since $\Delta(G) - \delta(G) \geq 2$, we suppose $u_{\Delta-1} \notin N_G(v)$. Let $S \subseteq E(G)$ be the set of edges which adjacent to u or v. Let $G^{**} = G - uu_{\Delta-1} + vu_{\Delta-1}$.

$$TI_f(G) = \sum_{uv \in E(G) \setminus S} f(d(u), d(v)) + \sum_{i=1}^{\Delta-1} f(\Delta, d(u_i)) + \sum_{i=1}^{\delta-1} f(\delta, d(v_i)) + f(\Delta, \delta).$$

$$\begin{aligned}
TI_f(G^{**}) &= \sum_{uv \in E(G) \setminus S} f(d(u), d(v)) + \sum_{i=1}^{\Delta-2} f(\Delta-1, d(u_i)) + \sum_{i=1}^{\delta-1} f(\delta+1, d(v_i)) \\
&\quad + f(d(u_{\Delta-1}), \delta+1) + f(\Delta-1, \delta+1).
\end{aligned}$$

$$\begin{aligned}
TI_f(G) - TI_f(G^{**}) &= \sum_{i=1}^{\Delta-1} [f(\Delta, d(u_i)) - f(\Delta-1, d(u_i))] - \sum_{i=1}^{\delta-1} [f(\delta+1, d(v_i)) - f(\delta, d(v_i))] \\
&\quad + f(\Delta, \delta) - f(\Delta-1, \delta+1) + f(\Delta-1, d(u_{\Delta-1})) - f(\delta+1, d(u_{\Delta-1})) \\
&\geq \sum_{i=1}^{\Delta-1} [f(\Delta, d(u_i)) - f(\Delta-1, d(u_i))] - \sum_{i=1}^{\delta-1} [f(\delta+1, d(v_i)) - f(\delta, d(v_i))] \\
&\quad + f(\Delta, \delta) - f(\Delta-1, \delta+1) \\
&\geq (\Delta-1)[f(\Delta, \Delta) - f(\Delta-1, \Delta)] - (\delta-1)[f(\delta+1, \delta) - f(\delta, \delta)] \\
&\quad + f(\Delta, \delta) - f(\Delta-1, \delta+1),
\end{aligned}$$

since $\Delta[f(\Delta, \Delta) - f(\Delta-1, \Delta)] - \delta[f(\delta+1, \delta) - f(\delta, \delta)] > 0$, then $TI_f(G) - TI_f(G^{**}) > f(\Delta-1, \Delta) - f(\Delta, \Delta) + f(\delta+1, \delta) - f(\delta, \delta) + f(\Delta, \delta) - f(\Delta-1, \delta+1)$.

Since $f(x, y)$ is the first good function, $h(x) = f(a, x) - f(b, x)$ is monotonically decreasing on x for any $a \geq b \geq 0$. Then for any $a_1 \geq a_2 \geq a_3 \geq a_4 \geq 0$, we have $f(a_1, a_3) - f(a_1, a_2) \geq f(a_3, a_4) - f(a_2, a_4)$. Thus we have $f(\Delta-1, \Delta) + f(\Delta, \delta) + f(\delta+1, \delta) \geq f(\Delta, \Delta) + f(\Delta-1, \delta) + f(\delta+1, \delta)$, and $f(\Delta-1, \delta) + f(\delta+1, \delta) + f(\Delta, \Delta) \geq f(\delta, \delta) + f(\Delta-1, \delta+1) + f(\Delta, \Delta)$. We have $TI_f(G) - TI_f(G^{**}) > 0$, which is contradict with that $TI_f(G)$ has the minimum value in G, thus by **Case 1** and **Case 2**, we know G is a almost regular graph, i.e., $\Delta(G) - \delta(G) \leq 1$. $\square$

Similarly, we also have

Theorem 2. *Let G be a connected (n,m) graph and $f(x, y)$ is the second good function. For any $a > b + 1 \geq 2$, $H(a, b) < 0$, where $H(a, b) = a[f(a, a) - f(a-1, a)] - b[f(b+1, b) - f(b, b)]$. If $TI_f(G)$ has the maximum value in G, then G is an almost regular graph, i.e., $\Delta(G) - \delta(G) \leq 1$.*

In the following, we suppose $f(x, y)$ is the first good function, and for any $a > b + 1 \geq 2$, $H(a, b) > 0$, where $H(a, b) = a[f(a, a) - f(a-1, a)] - b[f(b+1, b) - f(b, b)]$. Similar to the Corollary 1-4 of [12], we also have the following results.

Corollary 1. *Let G be a (chemical) tree with n vertices, $TI_f(G)$ has the minimum value in G, then $G \cong P_n$.*

Corollary 2. *Let G be a (chemical) unicyclic graph with n vertices, $TI_f(G)$ has the minimum value in G, then $G \cong C_n$.*

Corollary 3. *Let G be a (n, m) graph, $TI_f(G)$ has the minimum value in G, then G has $2m - n\lfloor \frac{2m}{n} \rfloor$ vertices of degree $\lfloor \frac{2m}{n} \rfloor + 1$, $n - n(\frac{2m}{n} - \lfloor \frac{2m}{n} \rfloor)$ vertices of degree $\lfloor \frac{2m}{n} \rfloor$.*

Corollary 4. *Let G be a (n, m) graph, $TI_f(G)$ has the minimum value in G. If $n|2m$, then G is a regular graph and $TI_f(G) = mf(\frac{2m}{n}, \frac{2m}{n})$.*

3. Concluding Remarks

If $f(x,y) = \sqrt{x^2 + y^2}$, corresponding chemical index is the Sombor index [11], it has been proof in [12] that the Sombor index meet the conditions of Theorem 1. Our results are the promotion of results of [12]. Our results are suitable for more chemical indices, for example, if $f(x,y) = x^2 + y^2$, corresponding chemical index is the forgotten index, we can easily proof the forgotten index index meet the conditions of Theorem 1. We use a unified way to consider the extremal values of VDB indices of (n,m)-graphs. We do not need to consider the chemical indices one by one.

Conflicts of Interest: "The author declares no conflict of interest."

References

[1] Bondy, J. A., & Murty, U. S. R. (2008) *Graph Theory*, Springer, New York.

[2] Gutman, I. (2013) Degree-based topological indices. *Croatica Chemica Acta, 86*, 351-361.

[3] Cruz, R., Pérez, T., & Rada, J. (2015) Extremal values of vertex-degree-based topological indices over graphs. *Journal of Applied Mathematics and Computing, 48*, 395-406.

[4] Cruz, R., & Rada, J. (2019) The path and the star as extremal values of vertex-degree-based topological indices among trees. *MATCH Communications in Mathematical and in Computer Chemistry, 82*, 715-732.

[5] Liu, H., Gutman, I., You, L., & Huang, Y. (2022) Sombor index: review of extremal results and bounds. *Journal of Mathmatical Chemistry, 60*, 771-798.

[6] Rada, J., & Bermudo, S. (2019) Is every graph the extremal value of a vertex-degree-based topological index? *MATCH Communications in Mathematical and in Computer Chemistry, 81*, 315-323.

[7] Rada, J., & Cruz, R. (2014) Vertex-degree-based topological indices over graphs. *MATCH Communications in Mathematical and in Computer Chemistry, 72*, 603-616.

[8] Raza, H., Nadeem, M. F., Ahmad, A., Ahsan, A. M., & Muhammad, A. (2021) Comparative study of valency-based topological indices for tetrahedral sheets of clay minerals, *Current Organic Synthesis, 18*, 711-718.

[9] Nadeem, M. F., Azeem, M., & Farman, I. (2021) Comparative study of topological indices for capped and uncapped carbon nanotubes. *Polycyclic Aromatic Compounds, 42*(7), 4666-4683.

[10] Nadeem, M. F., Imran, M., Siddiqui, H. M. A., Azeem, M., Khalil, A., & Ali. Y. (2021) Topological aspects of metal-organic structure with the help of underlying networks. *Arabian Journal of Chemistry, 14*(6), 103157, https://doi.org/10.1016/j.arabjc.2021.103157.

[11] Gutman, I. (2021) Geometric approach to degree-based topological indices: Sombor indices. *MATCH Communications in Mathematical and in Computer Chemistry, 86*, 11-16.

[12] Aashtab, A., Akbari, S., Madadinia, S., Noei, M., & Salehi, F. (2022) On the graphs with minimum Sombor index. *MATCH Communications in Mathematical and in Computer Chemistry, 88*, 553-559.

[13] Randić, M., (1975) On characterization of molecular branching. *Journal of the American Chemistry Society, 97*, 6609-6615.

[14] Estrada, E., Torres, L., Rodröguez, L., & Gutman, I. (1998) An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian Journal of Chemistry, 37A*, 849-855.

[15] Furtula, B., & Gutman, I. (2015) A forgotten topological index *Journal of Mathmatical Chemistry, 53*, 1184-1190.

[16] Gutman, I., & Trinajstić, N. (1972) Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons. *Chemical Physics Letters, 17*, 535-538.

[17] Gutman, I., Ruščić, B., Trinajstić, N., & Wilcox, C. F. (1975) Graph theory and molecular orbitals. XII. Acyclic polyenes. *Journal of Chemistry Physics, 62*, 3399-3405.

[18] Zhou, B., & Trinajstić, N. (2009) On a novel connectivity index. *Journal of Mathmatical Chemistry, 46*, 1252-1270.

[19] Furtula, B., Graovac, A., & Vukičević, D. (2010) Augmented Zagreb index. *Journal of Mathmatical Chemistry, 48*, 370-380.

[20] Gutman, I., Furtula, B., & Elphick, C. (2014) Three new/old vertex-degree-based topological indices. *MATCH Communications in Mathematical and in Computer Chemistry, 72*, 617-632.

[21] Vukičević, D., & Gašperov, M. (2010) Bond aditive modeling 1. Adriatic indices. *Croatica Chemica Acta, 83*, 243-260.

[22] Fajtlowicz, S. (1987) On conjectures of Graffiti-II. *Congressus Numerantium, 60*, 187-197.

[23] Vukičević, D., & Furtula, B. (2009) Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *Journal of Mathmatical Chemistry, 46*, 1369-1376.

[24] Eliasi, M., & Iranmanesh, A. (2011) On ordinary generalized geometric-arithmetic index. *Applied Mathematics Letters,* *24*, 582–587.

[25] Albertson, M. O. (1997) The irregularity of a graph. *Ars Combinatoria, 46*, 219-225.