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Extremal Graphs for Vertex–Degree–Based Indices with Given Matching Number

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Abstract

The question of finding extremal structures with respect to various graph indices has received a lot of attention. Among these indices, a large number are defined on vertex degrees. We consider a typical generalization of the vertex-degree based indices of a graph G defined by

$$I_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where $f(x, y)$ is symmetric bivariate function. We define a property concerning $f(x, y)$ and show that if $f(x, y)$ admits this property and G has a given matching number, then $I_f(G)$ is upper bounded by a graph with certain structure. Further, we show that the above property is admitted by a large number of degree-based indices. This means that the extremal structures of the graphs that have given matching number and attain the maximum values of these indices are the same.

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1 Introduction

In mathematical chemistry, particularly in QSPR/QSAR (quantitative structure-property/activity relationship) investigation, a large number of topological indices were introduced in an attempt to characterize the physico-chemical properties of molecules. In terms of graph theory, a molecular is conveniently modeled as a graph or chemical graph and, thus, a topological index can be measured by the distances between vertices, the graph spectra or the degrees of the vertices in the graph. Among these indices, the vertex-degree-based indices play important roles. Indeed, several dozens of vertex-degree-based indices have been introduced and extensively studied in the literature [16, 27, 40]. Probably the most studied are the Randić connectivity index R and the first and second Zagreb indices M_1 and M_2, respectively, which were introduced for the total π-energy of alternant hydrocarbons [14, 17].

A natural consideration in studying various degree-based indices is to find a general approach that can be applied to as many indices as possible in some way [25]. To this end, a general form of the degree-based indices of a graph G was introduced [32], which is represented as the sum of a function $f(d(u), d(v))$ among all the edges of G, i.e.,

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

where $f(x, y)$ is a real function with $f(x, y) = f(y, x) \geq 0$, $E(G)$ is the edge set of G and, for a vertex v of G, $d(v)$ is the degree of v. In the literature, $I_f(G)$ is also called the *connectivity function* [36] or *bond incident degree index* [3, 38].

In this paper, we focus on the maximum value of $I_f(G)$ for the graphs G with given matching number. In fact, for some particular functions $f(x, y)$, the extremal value of $I_f(G)$ received much attention in the literature. In particular, when $f(x, y) = x+y$ or $f(x, y) = xy$, $I_f(G)$ is known as the first Zagreb index $M_1(G)$ or second Zagreb index $M_2(G)$, respectively. In [8], Feng and Ilić showed that if G is a graph with matching number β (the size of a maximum matching), then

$$M_i(G) \leq \max\{M_i(H_1), M_i(H_\beta)\}, \quad i = 1, 2,$$

and the equality holds if and only if $G = H_1$ or $G = H_\beta$, where $H_1 = K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$ and $H_\beta = K_\beta \vee \overline{K_{n-\beta}}$.

Other particular forms of $I_f(G)$ were also considered. In [37], using the majorization of degree sequence, Yao et al. determined the extremal graphs for general sum-connectivity index where $f(x,y) = (x+y)^\alpha$ $(\alpha \geq 1)$ and the reformulated Zagreb index where $f(x,y) = (x+y-2)^\alpha$ among the class of trees, unicyclic graphs and bicyclic graphs with fixed matching number, respectively.

Motivated by the results above, we try to give a universal method to characterize the extremal structures of the graphs with given matching number that attain the maximum value of $I_f(G)$. To this end, we introduce the notion of the property $\mathcal{P}$ as follows:

Property $\mathcal{P}$: A real function $f(x,y)$ is called satisfying Property $\mathcal{P}$ if

$$f(x,y) > 0, \ \frac{\partial f(x,y)}{\partial x} \geq 0, \ \frac{d^2 f(x,x)}{dx^2} \geq 0 \text{ and } \frac{d^2 f(x,n-1)}{dx^2} \geq 0$$

for any $x \geq 1$ and $y \geq 1$.

For two positive integers i and β, define the graph H_i as

$$H_i = K_i \vee \left(K_{2\beta+1-2i} \cup \overline{K_{n-2\beta-1+i}}\right).$$

Let

$$\begin{aligned} Q(x) = &\frac{x(x-1)}{2} f(n-1,n-1) + x(2\beta-2x+1) f(2\beta-x,n-1) \\ &+ \frac{(2\beta-2x+1)(2\beta-2x)}{2} f(2\beta-x,2\beta-x) \\ &+ x(n-2\beta-1+x) f(x,n-1). \end{aligned}$$

We note that $Q(i) = I_f(H_i)$ for any $i \in \{1,2,\ldots,\beta\}$. In the following section, we show that if $f(x,y)$ satisfies Property $\mathcal{P}$ in the interval $[1,\beta] \times [1,\beta]$, then for any graph G with given matching number β, $I_f(G) \leq \max\{I_f(H_i) : i = 1,2,\ldots,\beta\}$. In addition, if $\frac{d^2Q(x)}{dx^2} \geq 0$ for $x \in [1,\beta]$, then $I_f(G) \leq \max\{I_f(H_1), I_f(H_\beta)\}$.

2 Main results

Let G be a simple graph. As usual, we use $V(G)$ and $E(G)$ to denote the vertex set and edge set of G. For $e \in E(G)$ (resp. $e \notin E(G)$), we denote by $G - e$ (resp. $G + e$) the graph obtained from G by removing (resp. adding) the edge e. A set M of edges in G is called a *matching* if M is independent. In particular, if a matching M has $|V(G)|/2$ edges, then we call M a *perfect matching.* The *matching number* $\beta(G)$ of G is the number of edges in a maximum matching.

A *component* of G is a maximal connected subgraph of G. For an integer $n > 0$, we denote by K_n and $\overline{K}_n$ the complete graph and the empty graph of n vertices, respectively. A component is called *even* (resp., *odd*) if it has an even (resp., odd) number of vertices. Let $o(G)$ be the number of odd components of G.

For two disjoint graphs G and H , we use $G \cup H$ to denote the *union* of G and H, that is, $V(G \cup H) = V(G) \cup V(H)$ and $E(G \cup H) = E(G) \cup E(H)$. Let $G \vee H$ denote the graph obtained from $G \cup H$ by adding an edge xy for any $x \in V(G)$ and $y \in V(H)$, that is, $V(G \vee H) = V(G) \cup V(H)$ and $E(G \vee H) = E(G) \cup E(H) \cup \{(x, y) : x \in V(G), y \in V(H)\}$.

Before proving the main result, we introduce some known results, which will be used in our forthcoming argument.

Theorem 1. *(Tutte-Berge formula, [28]) Let G be a graph with n vertices. Then*

$$\beta(G) = \frac{1}{2}(n - \max\{o(G - S) - |S| : S \subset V(G)\}). \qquad (2)$$

For a real function $f(x)$, in the following we also use $f'(x)$ and $f''(x)$ to denote $\frac{\mathrm{d}f(x)}{\mathrm{d}x}$ and $\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2}$, respectively, if no confusion can occur.

Lemma 1. *Let $f(x)$ and $g(x)$ be two real functions in the same domain. If $f(x) > 0$, $f'(x) \geq 0$, $f''(x) \geq 0$ and $g(x) > 0$, $g'(x) \geq 0$, $g''(x) \geq 0$, then $f(x)g(x)$ and $f(x) + g(x)$ are both convex. Further, if $f''(x) > 0$ or $g''(x) > 0$, then $f(x)g(x)$ is strictly convex.*

Proof. Let $h(x) = f(x).g(x)$ and $k(x) = f(x) + g(x)$. Then

$$h'(x) = f'(x)g(x) + f(x)g'(x), \quad h''(x) = f''(x)g(x) + f(x)g''(x) + 2f'(x)g'(x)$$

and

$$k'(x) = f'(x) + g'(x), k''(x) = f''(x) + g''(x).$$

Therefore, the lemma follows immediately. ■

Lemma 2. *Let G be a graph and $e \notin E(G)$. If $f(x, y)$ satisfies Property $\mathcal{P}$, then*

$$I_f(G) < I_f(G + e).$$

Proof. Since adding new edges in a graph increases some vertex degrees, the lemma obviously holds. ■

Based on the above two results, we now give our main result as follows:

Theorem 2. *Let G be a connected graph with n vertices and matching number β, $n > 2\beta$. If $f(x, y)$ is a symmetric bivariate function with Property $\mathcal{P}$, then*

$$I_f(G) \leq \max_{1\leq i\leq \beta} \{I_f(H_i)\}.$$

Further, a graph G attains the maximum value of $I_f(G)$ if and only if G is one in $\{H_1, H_2, \ldots, H_\beta\}$ that attains $\max_{1\leq i\leq \beta}\{I_f(H_i)\}$.

Proof. We may assume that G admits the maximum value of $I_f(G)$. By Theorem 1, G has a set S_0 of vertices such that

$$\beta = \frac{1}{2}(n - o(G - S_0) + |S_0|).$$

Denote $i = |S_0|$ and $q = o(G-S_0)$. Then $n-2\beta = q-i$. Let $G_1, G_2, \ldots, G_q$ be all the odd components of $G - S_0$. If $G - S_0$ has an even component, then we obtain a new graph G^* by adding an edge in G between a vertex of an even component and a vertex of an odd component of $G - S_0$, then $\beta(G^*) \geq \beta$ and $\beta(G^*) \leq \frac{1}{2}(n-o(G^*-S_0)+|S_0|) = \frac{1}{2}(n-o(G-S_0)+|S_0|) = \beta$. Further, by Lemma 2, $I_f(G^*) > I_f(G)$, which is a contradiction to the maximality of G. Therefore, $G-S_0$ does not contain any even component.

Let $|V(G_j)| = n_j$ for $j = 1, 2, \ldots, q$. We note that adding an edge in any component G_j or the subgraph induced by S_0 does not increase the matching number but increases the value of $I_f(G)$ by Lemma 2. So, again by the maximality of G, we have

$$G = K_i \vee (\bigcup_{1 \leq j \leq q} K_{n_j}).$$

Without loss of generality, we assume that $n_1 \geq n_2 \geq \ldots \geq n_q$.

Claim 1. $n_2 = n_3 = \cdots = n_q = 1$.

Proof. Recall that $n_1, n_2, \ldots, n_q$ are all odd. Suppose to the contrary that $n_2 \geq 3$. Let

$$G' = K_i \vee (K_{n_1+2} \cup K_{n_2-2} \cup \bigcup_{3 \leq j \leq q} K_{n_j}).$$

Let E^* be the set of edges incident with no vertex in $V(G_1 \cup G_2)$. We note that, for any $uv \in E^*$, $f(d_G(u), d_G(v)) = f(d_{G'}(u), d_{G'}(v))$. Recall that G is a connected graph and $f(x, y)$ is a nonnegative symmetric function. We may assume that $y \geq x \geq 1$. Then by (1) and a direct computation, we have

$$\begin{aligned} I_f(G) = {} & in_1 f(n_1 + i - 1, n - 1) + \tbinom{n_1}{2} f(n_1 + i - 1, n_1 + i - 1) \\ & + in_2 f(n_2 + i - 1, n - 1) + \tbinom{n_2}{2} f(n_2 + i - 1, n_2 + i - 1) \\ & + \sum_{uv \in E^*} f(d(u), d(v)) \end{aligned}$$

and

$$\begin{aligned} I_f(G') = {} & i(n_1 + 2) f(n_1 + i + 1, n - 1) + \tbinom{n_1+2}{2} f(n_1 + i + 1, n_1 + i + 1) \\ & + i(n_2 - 2) f(n_2 + i - 3, n - 1) + \tbinom{n_2-2}{2} f(n_2 + i - 3, n_2 + i - 3) \\ & + \sum_{uv \in E^*} f(d(u), d(v)). \end{aligned}$$

Thus,

$$\begin{aligned} I_f(G') - I_f(G) &= i(n_1+2)f(n_1+i+1, n-1) - in_1 f(n_1+i-1, n-1) \\ &\quad + i(n_2-2)f(n_2+i-3, n-1) - in_2 f(n_2+i-1, n-1) \\ &\quad + \binom{n_1+2}{2} f(n_1+i+1, n_1+i+1) - \binom{n_1}{2} f(n_1+i-1, n_1+i-1) \\ &\quad + \binom{n_2-2}{2} f(n_2+i-3, n_2+i-3) - \binom{n_2}{2} f(n_2+i-1, n_2+i-1). \end{aligned}$$

Let $S(x) = xf(x+i-1, n-1)$ and $T(x) = \frac{x(x-1)}{2} f(x+i-1, x+i-1)$. Recall that $f(x,y)$ satisfies Property $\mathcal{P}$, i.e.,

$$\frac{\partial f(x,y)}{\partial x} \geq 0, \frac{d^2 f(x,x)}{dx^2} \geq 0 \text{ and } \frac{d^2 f(x,n-1)}{dx^2} \geq 0$$

for any $x \geq 1$ and $y \geq 1$. Then we have $\frac{\mathrm{d}f(x,n-1)}{dx} \geq 0$, $\frac{d^2 f(x,n-1)}{dx^2} \geq 0$ and $\frac{df(x,x)}{dx} \geq 0$, $\frac{d^2 f(x,x)}{dx^2} \geq 0$. Note that $\frac{d}{dx}\left(\frac{x(x-1)}{2}\right) = x - \frac{1}{2} > 0$ and $\frac{d^2}{dx^2}\left(\frac{x(x-1)}{2}\right) = 1 > 0$. So by Lemma 1, $S(x)$ is convex and $T(x)$ is strictly convex. Therefore, we have

$$S(n_1+2) - S(n_1) \geq S(n_2) - S(n_2-2)$$

and

$$T(n_1+2) - T(n_1) > T(n_2) - T(n_2-2).$$

It follows that

$$\begin{aligned} I_f(G') - I_f(G) &= i(S(n_1+2) - S(n_1) + S(n_2-2) - S(n_2)) \\ &\quad + T(n_1+2) - T(n_1) + T(n_2-2) - T(n_2) \\ &> 0, \end{aligned}$$

which contradicts the maximality of G. ■

By Claim 1, $n_2 = n_3 = \cdots = n_q = 1$ and thus $n_1 = n - i - (q-1) = 2\beta - 2i + 1$. Therefore

$$G = H_i = K_i \vee \left(K_{2\beta-2i+1} \cup \overline{K_{n-2\beta+i-1}}\right),$$

where $1 \leq i \leq \beta$. As a result,

$$\begin{aligned} I_f(H_i) = &\tbinom{i}{2} f(n-1,n-1) + i(2\beta-2i+1) f(2\beta-i,n-1) \\ &+ \tbinom{2\beta-2i+1}{2} f(2\beta-i,2\beta-i) + i(n-2\beta+i-1) f(i,n-1) \end{aligned}$$

and we deduce that

$$I_f(G) \leq \max_{1\leq i\leq \beta} \{I_f(H_i)\}.$$

The second part of the theorem follows directly from the argument above, which completes our proof. ∎

The following corollary is a direct consequence of Theorem 2.

Corollary 1. *Let G be a connected graph, and let $f(x,y)$ be a real symmetric function satisfying Property $\mathcal{P}$ and $\frac{d^2Q(x)}{dx^2} \geq 0$ for any real number x with $1 \leq x \leq \beta < \frac{n}{2}$. Then*

$$I_f(G) \leq \max\{H_f(H_1), H_f(H_\beta)\}.$$

The equality holds if and only if $G = K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$ when $H_f(H_1) > H_f(H_\beta)$ or $G = K_\beta \vee \overline{K_{n-\beta}}$ when $H_f(H_1) < H_f(H_\beta)$ or both when $H_f(H_1) = H_f(H_\beta)$.

3 Application

In this section we apply Theorem 2 and Corollary 1 to some known degree-based indices. Recall that $Q(1) = H_f(H_1)$ and $Q(\beta) = H_f(H_\beta)$.

Example (Forgotten index $F(G)$). Let G be a connected graph of order n with $n \geq 10$ and matching number β. The Forgotten index of G is defined as [10]

$$F(G) = \sum_{uv\in E(G)} (d_u^2 + d_v^2).$$

Let r be the largest real root of

$$17x^3 + (-n-15)x^2 + (9-n)x + 3n^2 - n^3 - 4n = 0.$$

Then $F(G) \leq Q(\beta)$ if $\beta < r$ and $F(G) \leq Q(1)$ if $\beta > r$, where

$$\begin{aligned} Q(\beta) &= -\beta^4 + \beta^3 n + \beta n^3 - 3\beta n^2 + 3\beta n - \beta, \\ Q(1) &= 16\beta^4 - 32\beta^3 + 24\beta^2 - 10\beta + n^3 - 3n^2 + 4n. \end{aligned}$$

The two upper bounds are attained only by H_β or H_1, respectively.

Proof. The weight function of $F(G)$ is $f(x, y) = x^2 + y^2$. By a direct calculation, we have $\partial f(x, y)/\partial x = 2x \geq 0$, $d^2 f(x, x)/dx^2 = 4 > 0$ and $d^2 f(x, n-1)/dx^2 = 2 > 0$. This means that $f(x, y)$ satisfies Property $\mathcal{P}$. Further, again by a direct calculation, we have

$$\begin{aligned} Q(i) = {} & i(i-1)(n-1)^2 + i(2\beta - 2i + 1)\left((2\beta - i)^2 + (n-1)^2\right) \\ & + 2(2\beta - 2i + 1)(\beta - i)(2\beta - i)^2 + i(n - 2\beta + i - 1)\left(i^2 + (n-1)^2\right), \end{aligned}$$

$$\begin{aligned} \frac{dQ(i)}{di} = {} & -40\beta^3 + 12\beta^2(6i - 1) + 12\beta(1 - 4i)i + n^3 \\ & - 3n^2 + 3n\left(i^2 + 1\right) + 12i^3 - 6i^2 - 1, \end{aligned}$$

$$\frac{d^2 Q(i)}{di^2} = 72\beta^2 - 96\beta i + 12\beta + 6ni + 36i^2 - 12i.$$

Since $1 \leq i \leq \beta < \frac{n}{2}$, $12\beta - 12i \geq 0$. In addition, we have

$$72\beta^2 + 36i^2 \geq 12\sqrt{72}\beta i > 96\beta i.$$

Then we obtain $\frac{d^2 Q(i)}{di^2} > 0$. Hence, $Q(i)$ is strictly convex function. So by Corollary 1, we have

$$F(G) \leq \max\{Q(1), Q(\beta)\} \tag{3}$$

with equality only if $G = H_1$ or H_β. Further, we can see by a direct calculation that

$$Q(1) = 16\beta^4 - 32\beta^3 + 24\beta^2 - 10\beta + n^3 - 3n^2 + 4n,$$
$$Q(\beta) = -\beta^4 + \beta^3 n + \beta n^3 - 3\beta n^2 + 3\beta n - \beta.$$

Therefore,

$$\begin{aligned} Q(1) - Q(\beta) &= 17\beta^4 - \beta^3 n - 32\beta^3 + 24\beta^2 - \beta n^3 + 3\beta n^2 \\ &\quad - 3\beta n - 9\beta + n^3 - 3n^2 + 4n \\ &= (\beta - 1)\left(17\beta^3 + (-n-15)\beta^2 + (9-n)\beta - n^3 + 3n^2 - 4n\right). \end{aligned}$$

Let $H(x) = 17x^3 + (-n-15)x^2 + (9-n)x + (-n^3 + 3n^2 - 4n)$ and $H'(x) = 51x^2 - 10(2n+3)x + 9 - n = 0$. Then, by a direct calculation we obtain that for $n \geq 10$, there are two real roots

$$x_1 = \frac{1}{51}\left(-\sqrt{100n^2 + 351n - 234} + 10n + 15\right) < 0,$$
$$x_2 = \frac{1}{51}\left(\sqrt{100n^2 + 351n - 234} + 10n + 15\right) > 0.$$

Therefore, $H'(x) > 0$ in the interval $(-\infty, x_1)$, $H'(x) < 0$ in the interval (x_1, x_2) and $H'(x) > 0$ in the interval $(x_2, +\infty)$. Let $s(n) = \frac{1}{51}\left(\sqrt{100n^2 + 351n - 234} + 10n + 15\right)$. It is easy to see for $n \geq 4$, $x_2 \geq s(4) > 2$. Further, for $n \geq 10$, we have $H(0) = -n^3 + 3n^2 - 4n < 0$, which implies $H(x_2) < 0$, and $H(\frac{n}{2}) = \frac{1}{8}n(7n^2 - 10n + 4) > 0$ by a direct calculation. Recall that r is the largest root of $H(x) = 0$, meaning that r lies in $(x_2, \frac{n}{2})$ and, hence $r > x_2 > 2$. Therefore, r is the largest root of $Q(1) - Q(x) = 0$. As a result, we have $Q(1) < Q(\beta)$ if $\beta < r$ and $Q(1) > Q(\beta)$ if $\beta > r$. Combining with (3), the proof is completed. ■

In the following table we list some vertex-degree-based indices and give the calculating results for whether these indices satisfy Property $\mathcal{P}$ and further satisfy $\frac{d^2 Q(x)}{dx^2} \geq 0$ (in the table, the degree $d(v)$ of a vertex v is written by d_v for simplicity).

Table 1. Some vertex-degree-based indices, Property $\mathcal{P}$ and $Q''(i)$.

Indices	$f(d_u, d_v)$	$\mathcal{P}$	$Q''(i) \geq 0$
Augmented Zagreb index [9]	$AZI(G) = \sum_{uv \in E(G)} (\frac{d_u d_v}{d_u + d_v - 2})^3$	No	Yes
Atom-bond connectivity index [5]	$ABC(G) = \sum_{uv \in E(G)} (\frac{d_u + d_v - 2}{d_u d_v})^{1/2}$	No	No
Albertson index [2]	$Alb(G) = \sum_{uv \in E(G)} \lvert d_u - d_v \rvert$	No	No
Dharwad index [19]	$D(G) = \sum_{uv \in E(G)} \sqrt{d_u^3 + d_v^3}$	Yes	?
Extended Estrada index [26]	$EE(G) = \sum_{uv \in E(G)} (\frac{d_u}{d_v} + \frac{d_v}{d_u})/2$	No	?
First Zagreb index [17]	$Z_1(G) = \sum_{uv \in E(G)} d_u + d_v$	Yes	Yes
First hyper-Zagreb index [31]	$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$	Yes	Yes
Forgotten index [10]	$F(G) = \sum_{u \in V(G)} (d_u)^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$	Yes	Yes
First Gourava index [20]	$GO_1(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v)$	Yes	Yes
First hyper-Gourava index [21]	$HGO_1(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v)^2$	Yes	Yes
General Sum connectivity index [41]	$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha$, $\alpha \geq 1$	Yes	Yes
Generalized Randić index [4]	$R(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$, $\alpha \geq 1$	Yes	Yes
Geometric-arithmetic index [34]	$GA(G) = \sum_{uv \in E(G)} (\frac{2 d_u d_v}{d_u + d_v})^{1/2}$	No	Yes
Hyper F-index [11]	$HF(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2)^2$	Yes	Yes
Harmonic index [6]	$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$	No	Yes
Inverse sum Indeg Index [35]	$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$	No	Yes
Modified second Zagreb index [33]	$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}$	No	No
Modified Albertson index [39]	$Alb^*(G) = \sum_{uv \in E(G)} \lvert d_u^2 - d_v^2 \rvert$	No	No
Nirmala index [22]	$N(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v}$	No	No
Product connectivity Gourava index [23]	$PGO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_u + d_v)(d_u d_v)}}$	No	?
Randić connectivity index [30]	$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$	No	No
Reformulated Zagreb index [29]	$Z(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^2$	Yes	Yes
Reciprocal Randić index [12]	$RR(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v}$	No	Yes
Second Zagreb index [17]	$Z_2(G) = \sum_{uv \in E(G)} d_u d_v$	Yes	Yes
Sum connectivity index [18]	$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$	No	Yes
Sigma index [15]	$\sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2$	No	Yes
Sombor index [13]	$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$	Yes	?
Second Gourava index [20]	$GO_2(G) = \sum_{uv \in E(G)} (d_u + d_v) d_u d_v$	Yes	Yes
Second hyper-Gourava index [21]	$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) d_u d_v]^2$	Yes	Yes
Sum connectivity Gourava index [24]	$SGO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v + d_u d_v}}$	No	?
Second hyper-Zagreb index [7]	$HZ_2(G) = \sum_{uv \in E(G)} (d_u d_v)^2$	Yes	?
Y-index [1]	$Y(G) = \sum_{u \in V(G)} d_u^4 = \sum_{uv \in E(G)} (d_u^3 + d_v^3)$	Yes	Yes

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References

[1] A. Alameri, N. Al-Naggar, M. Al-Rumaima, M. Alsharafi, Y-index of some graph operations, *Int. J. Appl. Eng. Res.* **15** (2020) 173–179.

[2] M. O. Albertson, The irregularity of a graph, *Ars Comb.* **46** (1997) 219–225.

[3] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Discr. Appl. Math.* **238** (2018) 32–40.

[4] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[5] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: Modeling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[6] S. Fajtlowicz, On conjectures of Graffiti-II, *Congr. Num.* **60** (1987) 189–197.

[7] M. R. Farahani, M. R. R. Kanna, R. P. Kumar, On the hyper-Zagreb indices of nano-structures, *Asian Acad. Res. J. Multidis.* **3** (2016) 115–123.

[8] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* **23** (2010) 943–948.

[9] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* **48** (2010) 370–380.

[10] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[11] S. Ghobadi, M. Ghorbaninejad, On F-polynomial, multiple and hyper F-index of some molecular graphs, *Bull. Math. Sci. Appl.* **20** (2018) 36–43.

[12] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index,* Univ. Kragujevac, Kragujevac, 2008.

[13] I. Gutman, Geometric approach to degree-based topological indices: Sombor Indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[14] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[15] I. Gutman, M. Togan, A. Yurttas, A. S. Cevik, I. N. Cangul, Inverse problem for Sigma index, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 491–508.

[16] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors, vertex-degree-based topological indices, *J. Serb. Chem. Soc.* **78** (2013) 805–810.

[17] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[18] L. B. Kier, L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.

[19] V. R. Kulli, Dharwad index, *Int. J. Eng. Sci. Res. Technol.* **10** (2021) 17–21.

[20] V. R. Kulli, The Gourava indices and coindices of graphs, *Ann. Pure Appl. Math.* **14** (2017) 33–38.

[21] V. R. Kulli, On hyper-Gourava indices and coindices, *Int. J. Math. Arch.* **8** (2017) 116–120.

[22] V. R. Kulli, Nirmala index, *Int. J. Math. Trends Tech.* **67** (2021) 8–12.

[23] V. R. Kulli, The product connectivity Gourava index, *J. Comp. Math. Sci.* **8** (2017) 235–242

[24] V. R. Kulli, On the sum connectivity Gourava index, *Int. J. Math. Arch.* **8** (2017) 211–217.

[25] X. Li, Indices, polynomials and matrices – A unified viewpoint, *Invited talk at the 8th Slovenian Conf. Graph Theory*, Kranjska Gora, June 21–27, 2015.

[26] J. Li, Q. Lu, N. Gao, Bounds of the extended Estrada index of graphs, *Appl. Math. Comput.* **317** (2018) 143–149.

[27] B. Liu, I. Gutman, Upper bounds for Zagreb indices of connected graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 439–446.

[28] L. Lovász, M. D. Plummer, *Matching Theory*, Akadémiai Kiadó-North Holland, Budapest, 1986.

[29] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Divers.* **8** (2004) 393–399.

[30] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[31] G. H. Shirdel, H. Rezapour, A. M. Sayadi, The hyper-Zagreb index of graph operations, *Iran. J. Math. Chem.* **4** (2013) 213–220.

[32] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

[33] N. Trinajstić, On modified Zagreb M_2 index, *Reported at the MATH/CHEM/COMP 2002*, Dubrovnik, June 24–29, 2002.

[34] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[35] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta.* **83** (2010) 243–260.

[36] H. Wang, Functions on adjacent vertex degrees of trees with given degree sequence, *Central Eur. J. Math.* **12** (2014) 1656–1663.

[37] Y. Yao, M. Liu, K. C. Das, Y. Ye, Some extremal results for vertex-degree-based invariants, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 325–344.

[38] J. Ye, M. Liu, Y. Yao, K.C. Das, Extremal polygonal cacti for bond incident degree indices, *Discr. Appl. Math.* **257** (2019) 289–298.

[39] S. Yousaf, A. A. Bhatti, A. Ali, A note on the modified Albertson index, *Util. Math.* **117** (2020) 139–145.

[40] B. Zhou, I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.

[41] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.