MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 505-520
ISSN: 0340-6253
doi: 10.46793/match.88-3.505H

Extremal Graphs for Topological Index Defined by a Degree–Based Edge–Weight Function*

Zhoukun Hu, Luyi Li, Xueliang Li, Danni Peng

Center for Combinatorics and LPMC
Nankai University, Tianjin 300071, China

huzhoukun@mail.nankai.edu.cn, liluyi@mail.nankai.edu.cn,
lxl@nankai.edu.cn, pengdanni@mail.nankai.edu.cn

(Received November 17, 2021)

Abstract

For a simple graph G, d_u denotes the degree of a vertex u in G. Let $f(x,y)$ be a symmetric real function in two variables, and define the weight $w(e)$ of an edge $e = uv$ of G by $w(e) = f(d_u, d_v)$. Then the topological index $TI_f(G)$ of G defined by a degree-based edge-weight function $f(x,y)$ is given as $TI_f(G) = \sum_{uv\in E(G)} f(d_u, d_v)$. Let $f_1(x,y) = f(x+1,y) - f(x,y)$, $f_2(x,y) = f(x,y+1) - f(x,y)$, $f_{11} = (f_1)_1$, $f_{12} = (f_1)_2$ and $f_{111} = (f_{11})_1$. If $f(x,y)$ satisfies some of following properties: $f_1 > 0, f_{11} > 0, f_{12} \geq 0, f_{111} \geq 0$ and for any $x_1 + y_1 = x_2 + y_2$ with $|x_1 - y_1| > |x_2 - y_2|$, $f(x_1, y_1) > f(x_2, y_2)$, we obtain some upper bounds and lower bounds for the topological index $TI_f(G)$ and give some graphs of given order and size achieving the bounds. For graphs with small size, we characterize the graphs with maximal and minimal values of the index $TI_f(G)$.

1 Introduction

In this paper, we only consider simple, finite and undirected graphs. For a graph G, we use $V(G)$, $E(G)$, n and m to denote the vertex-set, the edge-set, the number of vertices and the number of edges of G, respectively. For a vertex $u \in G$, denote by $N_G(u)$ the neighbor set of a vertex u in G and by d_u the *degree* of u in G. We denote by Δ and δ

*Supported by NSFC No.12131013 and 11871034.

the *maximum degree* and *minimum degree* of G, respectively. A graph G is called *almost regular* if $\Delta - \delta \leq 1$. We use P_l to denote a path with length l. For k graphs $G_1, G_2, ..., G_k$, the union $G_1 \cup G_2 \cup \cdots \cup G_k$ is the graph with vertex-set $V(G_1) \cup V(G_2) \cup \cdots \cup V(G_k)$ and edge-set $E(G_1) \cup E(G_2) \cup \cdots \cup E(G_k)$. In particular, denote by $kG = G_1 \cup G_2 \cup \cdots \cup G_k$ if $G = G_1 = G_2 = \cdots = G_k$. The join $G \vee H$ of two graphs G and H is the graph obtained by joining edges between each vertex of G to all vertices of H. For terminology and notation not defined here, we refer the reader to [3, 16].

As we all know, there are many degree-based topological indices or chemical indices which are useful in chemistry [1, 16], and each of them is defined as the sum of the edge-weights defined by a symmetric real function $f(x, y)$, for examples, the Zagreb indices by functions $f(x, y) = x + y$ and $f(x, y) = xy$, the Randić index [13] by the function $f(x, y) = \frac{1}{\sqrt{xy}}$, and the ABC-index [5] by the function $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$, etc. For more functions, we refer to [7, 9, 11].

For topological indices defined by summing up the vertex-weights, Yao et al. in [17] and Tomescu in [14, 15] studied the so-called vertex-degree function-index $H_f(G)$, which is defined as $H_f(G) = \sum_{v \in V(G)} f(d_v)$, where $f(x)$ is a real function of one variable x. Yao et al., Tomescu, and the present authors in [10] got some extremal results for the index $H_f(G)$. In this paper, we will study the topological index defined by summing up the edge-weights of a graph with edge-weights given by a symmetric real function $f(x, y)$, which was introduced by Gutman in [8]. The definition is stated as follows.

Definition 1.1. *Let G be a graph and $f(x, y)$ be a symmetric real function. Define the weight $w(e)$ of an edge $e = uv$ in G by $f(d_u, d_v)$. Then the topological index $TI_f(G)$ of G with edge-weight function $f(x, y)$ is defined as*

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

Cruz and Rada studied the topological index $TI_f(G)$. In [12] Rada and Cruz obtained some extremal results for graphs with n vertices but without isolated vertices, with no restriction on the number of edges. Later in [4] Cruz and Rada obtained some extremal results for trees with the weight function $f(x, y)$ being an exponential type. Now we will study extremal problem for graphs with n vertices and m edges.

Before proceeding, we need the following notation and terminology. For a family $\mathcal{G}$ of graphs, we call a graph G *minimal* in $\mathcal{G}$ if $TI_f(G) = \min_{H\in\mathcal{G}} TI_f(H)$, and *maximal* in $\mathcal{G}$ if $TI_f(G) = \max_{H\in\mathcal{G}} TI_f(H)$. For a symmetric real function $f(x,y)$, let $f_1(x,y) = f(x+1,y) - f(x,y)$ and $f_2(x,y) = f(x,y+1) - f(x,y)$. So we have $(f_1)_1(x,y) = f_1(x+1,y) - f_1(x,y) = f(x+2,y) - f(x+1,y) - f(x+1,y) + f(x,y)$. Let $f_{11} := (f_1)_1$ and $f_{12} := (f_1)_2$. We say that $f \geq (>,=,<,\leq)\ 0$ if $f(x,y) \geq (>,=,<,\leq)\ 0$ for any x and y. $f(x,y)$ is called *(strictly) monotonically increasing* if f_1 is non-negative(positive). Notice that if $f(x,y)$ is partial differentiable and $\frac{\partial f}{\partial x}$ is positive (non-negative), then f_1 is positive (non-negative). Sometimes we need the convexity of a real function. $f(x,y)$ is called *convex* if for any (x_1,y_1), (x_2,y_2) and $\mu \in (0,1)$, $f(\mu x_1+(1-\mu)x_2, \mu y_1+(1-\mu)y_2) \leq \mu f(x_1,y_1) + (1-\mu)f(x_2,y_2)$. Notice that the convexity of f implies $f_{11} \geq 0$. In this paper, we mainly consider symmetric real functions $f(x,y)$ with $f_{11} > 0$. The following properties of a function frequently appear in some of our results. We say that a function $f(x,y)$ has the **property** P (P') if for any $x_1 + y_1 = x_2 + y_2$ and $|x_1 - y_1| > |x_2 - y_2|$, $f(x_1,y_1) >\ (<)\ f(x_2,y_2)$. It is not difficult to see that a symmetric and convex function has the property P.

The following observations are easily seen.

Proposition 1.2. *Let G be a graph and $f(x,y)$ be a symmetric real function.*

1. *If $G_1, G_2, \ldots, G_t$ are the connected components of G, then $TI_f(G) = \sum_{i=1}^{t} TI_f(G_i)$.*
2. *If there is a function $g(x)$ such that $f(x,y) = g(x) + g(y)$ and $h(x) = xg(x)$, then*

$$TI_f(G) = \sum_{uv\in E(G)} (g(d_u) + g(d_v)) = \sum_{v\in V(G)} d_v g(d_v) = H_h(G).$$

3. *If $f_1 \geq 0$, then $TI_f(G) \geq TI_f(G - uv)$ for any $uv \in E(G)$.*

Our results focus on the maximal graphs and minimal graphs among the graphs with n vertices and m edges. For the minimal graphs, we get a general lower bound.

Theorem 1.3. *Let n and m be integers such that $n \geq 2$ and $1 \leq m \leq n(n-1)/2$. If $f(x,y)$ is convex and partial differentiable with $\frac{\partial f}{\partial x} \geq 0$, then we have*

$$TI_f(G) \geq mf(2m/n, 2m/n),$$

the bound is sharp since all regular graphs can achieve the lower bound.

Although this lower bound is a rough estimate, it can also be achieved by regular graphs. However, by a deeper analysis, we can get a clearer characterization for the minimal graphs. We give two better results under the condition that the size m is small. Notice that these minimal graphs are all almost regular graphs.

Theorem 1.4. *Let n and m be integers such that $n \geq 2$ and $1 \leq m \leq n/2$. If $f(x,y)$ is symmetric and $f_1 > 0$, then for any graph G with n vertices and m edges, we have $TI_f(G) \geq mf(1,1)$, and the equality holds if and only if $G = mK_2 \cup (n-2m)K_1$.*

Theorem 1.5. *Suppose n and m are integers such that $n \geq 2$ and $n/2 \leq m \leq n-1$. Let $\mathcal{G}(n,m)$ be the family of graphs with n vertices and m edges. If $f(x,y)$ satisfies that $f_1 > 0$, $f_{11} > 0$, $f_{12} \geq 0$ and $f(1,3) > f(2,2)$, then every minimal graph in $\mathcal{G}(n,m)$ is an almost regular graph. Moreover, if $f(1,1) + f(2,2) = 2f(1,2)$, then every almost regular graphs is also a minimal graph in $\mathcal{G}(n,m)$.*

For a non-trivial component G_1 of graph G, a vertex v is a *universal vertex* in G_1 if $d_v = |V(G_1)| - 1$. In this situation, the maximal graphs have following property.

Theorem 1.6. *Suppose n and m are integers such that $n \geq 2$ and $1 \leq m \leq n(n-1)/2$. Let $\mathcal{G}(n,m)$ be the family of graphs with n vertices and m edges. If $f(x,y)$ has the property P and satisfies that $f_1 > 0$ and $f_{11} > 0$, then the maximal graphs in $\mathcal{G}(n,m)$ have exactly one non-trivial component, and the component has a universal vertex.*

When $m \leq n-1$, we can prove that the unique maximal graph is the union of a star and some isolated vertices.

Theorem 1.7. *Suppose n and m are integers such that $n \geq 2$ and $1 \leq m \leq n-1$. Let G be a graph with n vertices and m edges. If $f(x,y)$ has the property P and satisfies $f_1 > 0$, then $TI_f(G) \leq mf(1,m)$, and the equality holds if and only if $G = K_{1,m} \cup (n-m-1)K_1$.*

When m is larger, we find the unique maximal graph among all connected graphs.

Theorem 1.8. *Suppose n and m are integers such that $n \geq 3$ and $n-1 \leq m \leq 2n-3$. Let $\gamma = m-n+1$ and $\mathcal{G}^c(n,m)$ be the family of connected graphs with n vertices and m edges. If $f(x,y)$ has the property P and satisfies that $f_1 > 0$, $f_{11} > 0$ and $f_{111} \geq 0$, then we have that for any $G \in \mathcal{G}^c(n,m)$, $TI_f(G) \leq (n-\gamma-2)f(n-1,1) + \gamma f(n-1,2) + \gamma f(\gamma+1,2) + f(n-1,\gamma+1)$, and the equality holds if and only if $G = K_1 \vee (K_{1,\gamma} \cup (n-\gamma-2)K_1)$.*

The forgotten index [6] is defined as $F(G) = \sum_{uv\in E(G)}(d_u^2 + d_v^2)$ with edge-weight function $f(x,y) = x^2 + y^2$, which has the property P and satisfies that $f_1 > 0$, $f_{11} > 0$, $f_{12} \geq 0$ and $f_{11} \geq 0$. Thus by Theorems 1.3 to 1.8, we can get the maximal graph and the minimal graph immediately.

Moreover, some of our theorems are suitable for more indices. For instance, the Sombor index [9] is defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}$ with edge-weight function $f(x,y) = \sqrt{x^2+y^2}$, which has the property P and satisfies that $f_1 > 0$ and $f_{11} > 0$, Thus, Theorems 1.3, 1.4, 1.6 and 1.7 can be applied to the Sombor index. Moreover, Theorem 1.4 can be applied to more indices, such as the *the general Randić index* [2] with edge-weight function $f(x,y) = (xy)^\alpha$ by setting $\alpha \geq 1$.

Similar results hold for the edge-weight function $f(x,y)$ has the property P' and satisfying that $f_1 < 0$ and $f_{11} < 0$. In this case, we can get the extremal graphs by similar arguments.

2 Preliminaries

When we find the extremal graphs, we always start from a graph G and get another graph G' by some operations such that $m(G) = m(G')$ and $n(G) = n(G')$. In the process of comparing the values of the index of these two graphs, we always use d_x and $N(x)$ to denote the degree of x and the neighborhood of x in G, respectively.

The following lemma can be regarded as the binary function version of the *Jensen Inequality*, which is significant for the estimate of the lower bound and the minimal graphs.

Lemma 2.1. *If $f(x,y)$ is convex in a convex set D, then for any integer k, $i \in \{1,2,\ldots,$ $k\}$, $(x_i,y_i) \in D$, $u_i > 0$ and $\sum_{i=1}^k \mu_i = 1$,*

$$f\left(\sum_{i=1}^k \mu_i x_i, \sum_{i=1}^k \mu_i y_i\right) \leq \sum_{i=1}^k \mu_i f(x_i,y_i).$$

Proof. By induction on k, when $k = 1,2$, the inequality holds obviously. Suppose that for $k = t-1$, $t \geq 3$, the inequality holds. Then for $k = t$,

$$f\left(\sum_{i=1}^k \mu_i x_i, \sum_{i=1}^k \mu_i y_i\right) = f\left((1-u_k)\sum_{i=1}^{k-1}\frac{\mu_i x_i}{1-\mu_k} + \mu_k x_k, (1-u_k)\sum_{i=1}^{k-1}\frac{\mu_i y_i}{1-\mu_k} + \mu_k y_k\right)$$

$$\leq (1-u_k) f\left(\sum_{i=1}^{k-1} \frac{\mu_i x_i}{1-\mu_k}, \sum_{i=1}^{k-1} \frac{\mu_i y_i}{1-\mu_k}\right) + \mu_k f(x_k, y_k)$$
$$\leq (1-u_k) \sum_{i=1}^{k-1} \frac{\mu_i}{1-\mu_k} f(x_i, y_i) + \mu_k f(x_k, y_k)$$
$$= \sum_{i=1}^{k-1} \mu_i f(x_i, y_i) + \mu_k f(x_k, y_k) = \sum_{i=1}^{k} \mu_i f(x_i, y_i),$$

the first inequality holds by the definition of convex function, and the second inequality holds by the induction hypothesis. The proof is thus complete. ■

In a graph, we say a path $P_k = v_0 v_1 \ldots v_k$ is a *pendant path* if $d_{v_i} = 2$ for any i with $1 \leq i \leq k-1$ and $d_{v_k} = 1$, and v_0 is called the origin vertex of the pendant path.

Lemma 2.2. *Suppose $k, l \geq 1$ are integers, and G is a graph containing two pendant paths $P_k = wv_1 \ldots v_k$ and $P_l = wu_1 \ldots u_l$ such that $d_w \geq 3$ (see Figure 1). If $G' = G + u_1 v_k - wu_1$, then $TI_f(G') < TI_f(G)$ provided that $f_1 > 0$ and $f(2,2) < \min\{f(1,3), \frac{f(2,1)+f(2,3)}{2}\}$.*

Proof. Let $w = v_0$. Since $f(x+1, y) > f(x, y)$, we have that $TI_f(G') - TI_f(G)$ is equal to

$$\sum_{x \in N(w) \setminus u_1} [f(d_x, d_w - 1) - f(d_x, d_w)] + f(d_{v_{k-1}}, 2) - f(d_{v_{k-1}}, 1) + f(2,2) - f(d_w, 2)$$
$$< f(d_{v_{k-1}}, 2) - f(d_{v_{k-1}}, 1) + f(2,2) - f(d_w, 2).$$

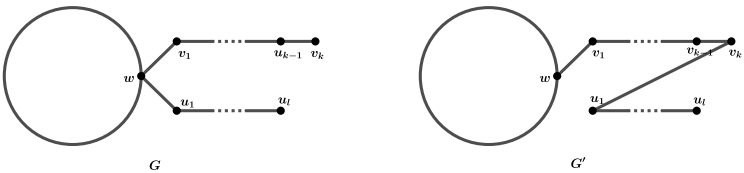

Figure 1. The graphs G and G' in Lemma 2.2.

If $k-1 \geq 1$, then $d_{v_{k-1}} = 2$. We can conclude that $f(2,2) - f(2,1) + f(2,2) - f(2, d_w) \leq f(2,2) - f(2,1) + f(2,2) - f(2,3) < 0$. If $k - 1 = 0$, then $f(d_w, 2) - f(d_w, 1) + f(2,2) - f(d_w, 2) = -f(d_w, 1) + f(2,2) \leq -f(3,1) + f(2,2) < 0$. It shows that $TI_f(G') - TI_f(G) < 0$ holds for both two cases. The proof is thus complete. ■

Applying Lemma 2.2, we get the unique minimal tree among all trees of order n.

Lemma 2.3. *Suppose T is a tree with n vertices. If $f(x,y)$ satisfies that $f_1 > 0$ and $f(2,2) < \min\{f(1,3), \frac{f(2,1)+f(2,3)}{2}\}$, then $TI_f(T) \geq 2f(1,2) + (n-1)f(2,2)$, and the equality holds if and only if T is the path P_{n-1}.*

Proof. By a contradiction. Suppose T is a minimal graph among trees with n vertices and T is not a path. Then T contains a vertex of degree at least three. Moreover, since T satisfies the condition of Lemma 2.2, we can get a new tree T' with $TI_f(T') < TI_f(T)$, which contradicts the minimality of T. The proof is thus complete. ■

Lemma 2.4. *Suppose $\mathcal{G}^c(n,n)$ is the family of connected graphs with n vertices and n edges. If $f(x,y)$ satisfies that $f_1 > 0$, $f_{11} > 0$, $f_{12} \geq 0$, and $f(1,3) > f(2,2)$, then for any graph $G \in \mathcal{G}^c(n,n)$, $TI_f(G) \geq nf(2,2)$, and the equality holds if and only if G is a cycle.*

Proof. Suppose G is a minimal graph in $\mathcal{G}^c(n,n)$. Since $|E(G)| = |V(G)| = n$ and G is connected, G contains a unique cycle. If G is not a cycle itself, then by Lemma 2.2, G is a cycle C with some paths pendant on different origin vertices. That is, $\Delta(G) \leq 3$. Let P^1 be a pendant path in G with the origin vertex z in C and the leaf vertex, say y. Then, $d_z = 3$ and $d_y = 1$. We denote the neighbor of y by y'. It follows that $d_{y'}$ is either 2 or 3. We distinguish the following cases to discuss.

Case 1. There exists a neighbor w of z in the cycle C with degree 2.

Then we delete the edge zw in $E(C)$ and add the edge wy. Thus we get a new graph $G_1 \in \mathcal{G}^c(n,n)$; see Figure 2.

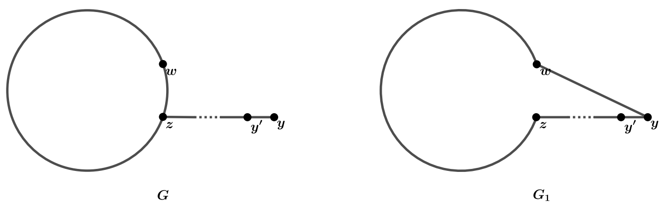

Figure 2. The graphs G and G_1 for Case 1 in the proof of Lemma 2.4.

Then,

$$TI_f(G) - TI_f(G_1) = \sum_{v \in N(z)\backslash\{w,y\}} [f(d_v, 3) - f(d_v, 2)] + f(3, 2) + f(1, d_{y'}) - f(2, 2) - f(2, d_{y'}) > 0,$$

which contradicts the minimality of G.

Case 2. All the neighbors of z in the cycle C have degree 3.

Then there exists another pendant path P^2 in H with the origin vertex $w \in N(z)$ and the leaf vertex, say l. We denote the neighbor of l by l'. It follows that $d_{l'}$ is either 2 or 3. Deleting the edge wz and adding the edge yl, we get a new graph G_2; see Figure 3. Then,

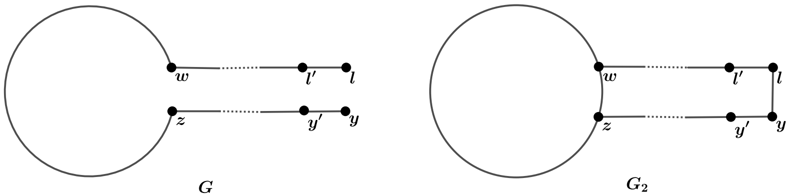

Figure 3. The graphs G and G_2 for Case 2 in the proof of Lemma 2.4.

$$\begin{aligned} TI_f(G) - TI_f(G_2) = & \sum_{v \in N(z)\backslash\{w,y\}} [f(d_v, 3) - f(d_v, 2)] + \sum_{v \in N(w)\backslash\{z,l\}} [f(d_v, 3) - f(d_v, 2)] \\ & + f(3, 3) + f(1, d_{y'}) + f(1, d_{l'}) - f(2, d_{y'}) - f(2, d_{l'}) - f(2, 2) \\ & > f(3, 3) - f(2, 2) - f_1(1, d_{l'}) - f_1(1, d_{y'}). \end{aligned}$$

Note that $2 \le d_{y'}, d_{l'} \le 3$, $f_{11} > 0$, $f_{12} \ge 0$ and $f(1, 3) > f(2, 2)$. So,

$$\begin{aligned} & TI_f(G) - TI_f(G_2) > f(3, 3) - f(2, 3) + f(3, 2) - f(2, 2) - f_1(1, d_{l'}) - f_1(1, d_{y'}) \\ & = f_1(2, 3) + f_1(2, 2) - f_1(1, d_{l'}) - f_1(1, d_{y'}) \ge f_1(2, 3) + f_1(2, 2) - 2f_1(1, 3) \\ & = f(3, 3) + 2f(1, 3) - f(2, 2) - 2f(2, 3) > f(3, 3) - 2f(2, 3) + f(1, 3) \\ & = f_1(2, 3) - f_1(1, 3) > 0. \end{aligned}$$

Hence, we find a graph $G_2 \in \mathcal{G}^c(n, n)$ such that $TI_f(G) > TI_f(G_2)$, a contradiction. Therefore, the minimal graph G is a cycle itself. The proof is now complete. ■

Next we consider the number of non-trivial components in the maximal graphs and get the following result.

Lemma 2.5. *Suppose n and m are integers such that $n \geq 2$ and $1 \leq m \leq n(n-1)/2$. Let $\mathcal{G}(n,m)$ be the family of graphs with n vertices and m edges. If $f(x,y)$ is symmetric and $f_1 > 0$, then the maximal graphs in $\mathcal{G}(n,m)$ have exactly one non-trivial component.*

Proof. Suppose to the contrary that a maximal graph G in $\mathcal{G}(n,m)$ contains at least two non-trivial components. Choose two vertices v_1 and v_2 from two distinct non-trivial components of G. Then we have that $d_{v_1} \geq 1$ and $d_{v_2} \geq 1$. Contracting v_1 and v_2 and adding an isolated vertex w, we get a new graph $G' \in \mathcal{G}(n,m)$ with less non-trivial components; see Figure 4.

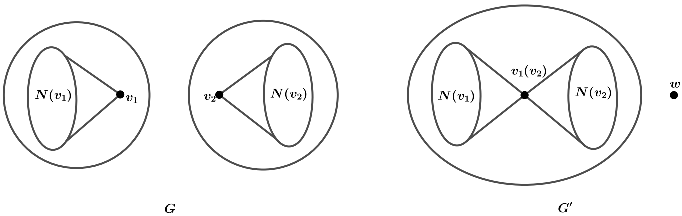

Figure 4. The graphs G and G' in the proof of Lemma 2.5.

Then we have $TI_f(G') - TI_f(G)$ is equal to

$$\sum_{x \in N(v_1)} [f(d_{v_1} + d_{v_2}, d_x) - f(d_{v_1}, d_x)] + \sum_{x \in N(v_2)} [f(d_{v_1} + d_{v_2}, d_x) - f(d_{v_2}, d_x)] > 0,$$

which contradicts of the maximality of G. Thus the maximal graphs in $\mathcal{G}(n,m)$ have at most one non-trivial component. ■

Before considering the maximal graphs with larger size, we introduce a previous result on the vertex-degree function-index from [15]. Let $f_1(x) = f(x+1) - f(x)$. $f(x)$ is convex if $f_1(x+1) \geq f_1(x)$. In fact, we use a weaker version of Theorem 2.3 of [15].

Lemma 2.6. *[15] Suppose n and m are integers such that $n \geq 2$ and $1 \leq m \leq n-1$. Let G be a graph with n vertices and m edges. If $f(x)$ and $f_1(x)$ are both convex, then*

$$H_f(G) \leq f(m) + mf(1) + (n-m-1)f(0),$$

and $G = K_{1,m} \cup (n-m-1)K_1$ can achieve this bound.

3 Proofs of Theorems 1.3, 1.4 and 1.5

In this section we will give the proofs of three results on the lower bounds.

Proof of Theorem 1.3: Assume that the two endpoints of e are $r(e)$ and $l(e)$ for any edge $e \in E(G)$. It follows from the definition of $TI_f(G)$ that

$$TI_f(G) = \sum_{e \in E(G)} f(d_{r(e)}, d_{l(e)}) \; .$$

Let $\sum_1 = \sum_{e \in E(G)} d_{r(e)}$ and $\sum_2 = \sum_{e \in E(G)} d_{l(e)}$. Then using Lemma 2.1, we have

$$TI_f(G) \geq mf\left(\sum_1 /m, \sum_2 /m\right).$$

By the symmetry and convexity of $f(x,y)$, we have

$$f\left(\frac{\sum_1}{m}, \frac{\sum_2}{m}\right) = \left[\frac{1}{2}f\left(\frac{\sum_1}{m}, \frac{\sum_2}{m}\right) + \frac{1}{2}f\left(\frac{\sum_2}{m}, \frac{\sum_1}{m}\right)\right] \geq f\left(\frac{\sum_1 + \sum_2}{2m}, \frac{\sum_1 + \sum_2}{2m}\right).$$

Notice that $\sum_1 + \sum_2 = \sum_{e \in E(G)}(d_{r(e)} + d_{l(e)}) = \sum_{v \in V(G)} d_v^2$. Then

$$f\left(\frac{\sum_1}{m}, \frac{\sum_2}{m}\right) \geq f\left(\frac{\sum_1 + \sum_2}{2m}, \frac{\sum_1 + \sum_2}{2m}\right) = f\left(\frac{\sum_{v \in V(G)} d_v^2}{2m}, \frac{\sum_{v \in V(G)} d_v^2}{2m}\right).$$

From the Cauchy-Schwarz inequality and the monotonicity of $f(x,y)$, we have

$$f\left(\frac{\sum_{v \in V(G)} d_v^2}{2m}, \frac{\sum_{v \in V(G)} d_v^2}{2m}\right) \geq f\left(\frac{4m^2}{2mn}, \frac{4m^2}{2mn}\right) = f\left(\frac{2m}{n}, \frac{2m}{n}\right).$$

Combining the inequalities above, we can deduce that $TI_f(G) \geq mf(2m/n, 2m/n)$, completing the proof. ■

Proof of Theorem 1.4: Suppose G is a minimal graph. We assert that $\Delta(G) \leq 1$. If not, then suppose there is a vertex $u \in V(G)$ of degree at least 2. Since $\sum_{v \in V(G)} d_v = 2m \leq n$, there exists an isolated vertex $w \in V(G)$. Suppose $x \in N(u)$, deleting ux and adding wx, we obtain a new graph G'. Then

$$TI_f(G) - TI_f(G') = \sum_{v \in N(u) \backslash x} [f(d_u, d_v) - f(d_u - 1, d_v)] + f(d_u, d_x) - f(1, d_x) > 0,$$

which contradicts the minimality of G. Consequently, the degree of each vertex in G is at most 1, which means that G is the union of a matching and some isolated vertices. The proof is thus complete. ■

Proof of Theorem 1.5: Suppose G is a minimal graph in $\mathcal{G}(n,m)$. First, we claim that there is no isolated vertices in G. Otherwise, suppose v is an isolated vertex. Since $m \geq n/2$, there is a vertex u with degree at least 2. Suppose $x \in N(u)$, deleting ux and adding vx, we get a new graph $G' \in \mathcal{G}(n,m)$. Then

$$TI_f(G) - TI_f(G') = \sum_{v \in N(u)\backslash x} [f(d_u,d_v) - f(d_u-1,d_v)] + f(d_u,d_x) - f(1,d_x) > 0,$$

which contracts the minimality of G. Thus G contains no isolated vertices.

Suppose $H_1, H_2, \ldots, H_s$ are the components of G containing cycles and $K_1, K_2, \ldots, K_t$ are the rest components in G that do not contain cycles. Since G contains no isolated vertices, each component has at least 2 vertices. By Lemma 2.3 and Proposition 1.2, the t connected components K_i of G that do not contain cycles must be paths. If $s = 0$, then G is almost regular.

It remains to show that G is almost regular for $s \geq 1$. Moreover, since $|E(H_i)| \geq |V(H_i)|$ for any i and $|E(K_j)| = |V(K_j)| - 1$ for any j, we have

$$m = \sum_{i=1}^{s} |E(H_i)| + \sum_{j=1}^{t} |E(K_j)| \geq \sum_{i=1}^{s} |V(H_i)| + \sum_{j=1}^{t} (|V(K_j)| - 1) = n - t.$$

Thus, $t \geq 1$.

If $t = 1$, we know that $|E(H_i)| = |V(H_i)|$ for any i. Applying Lemma 2.4, H_i is a cycle for any i. Thus, G is almost regular. If $t \geq 2$, we assert that H_i is a cycle for all $1 \leq i \leq s$. Otherwise, there is a cycle C and a vertex $w \in C$ in some connected component H_i such that $d_w \geq 3$. Pick an edge $zw \in E(C)$. We choose a leaf $x \in K_1$ and a leaf $y \in K_2$. In both two cases, x, y are not adjacent. Assume that x' and y' are neighbor of x and y, respectively. We obtain a new graph $G' \in \mathcal{G}(n,m)$ from G by adding xy and deleting wz; see Figure 5. Then

$$\begin{aligned}
TI_f(G) - TI_f(G') = & \sum_{v \in N(w)\backslash z} [f(d_w,d_v) - f(d_w-1,d_v)] + \sum_{v \in N(z)\backslash w} [f(d_z,d_v) - f(d_z-1,d_v)] \\
& + f(d_{x'},1) + f(d_{y'},1) - f(d_{x'},2) - f(d_{y'}2) + f(d_z,d_w) - f(d_x+1,f_y+1) \\
= & \sum_{v \in N(w)\backslash z} f_1(d_w-1,d_v) + \sum_{v \in N(z)\backslash w} f_1(d_z-1,d_v) \\
& - f_1(1,d_{x'}) - f_1(1,d_{y'}) + f(d_z,d_w) - f(2,2).
\end{aligned}$$

Recall that $d_w \geq 3$, $d_z \geq 2$, $d_{x'} \leq 2$ and $d_{y'} \leq 2$. Using the property that $f_{12} \geq 0$ and $f_{11} > 0$, we have that $TI_f(G) - TI_f(G')$ is at least

$$f_1(d_w - 1, 2) + f_1(d_z - 1, 2) - f_1(1, 2) - f_1(1, 2) + f(d_z, d_w) - f(2, 2) > 0,$$

which contradicts the minimality of G. Thus, H_i is a cycle for all i with $1 \leq i \leq s$ and K_j is a path for all j with $1 \leq j \leq t$ in G.

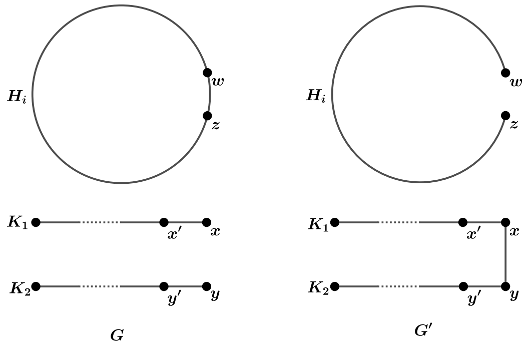

Figure 5. The graphs G and G' for the case that $s \geq 1$ and $t \geq 2$ in the proof of Theorem 1.5.

Finally, since the degree of each vertex in G is 1 or 2, G has exactly $2m-n$ vertices with degree 2 and $2n - 2m$ vertices with degree 1. Suppose G has r components isomorphic to P_1. Then there are $(n - m - r)$ path-components whose lengths are at least 2. Thus

$$\begin{aligned} TI_f(G) &= rf(1,1) + 2(n-m-r)f(1,2) + (3m-2n+r)f(2,2) \\ &= 2(n-m)f(1,2) + (3m-2n)f(2,2) + r[f(1,1) - 2f(1,2) + f(2,2)]. \end{aligned}$$

Note that from $f_{12} \geq 0$ one can deduce that $f(1,1) - 2f(1,2) + f(2,2) \geq 0$. If $f(1,1) + f(2,2) = 2f(1,2)$, then $TI_f(G)$ is exactly a constant for any G with the property. Thus every almost regular graph is a minimal graph in $\mathcal{G}(n,m)$.

The proof is now complete. ∎

4 Proofs of Theorems 1.6, 1.7 and 1.8

In this section we will give the proofs of three results on the upper bounds.

Proof of Theorem 1.6: Suppose G is a maximal graph in $\mathcal{G}(n,m)$. By Lemma 2.5, G has only one non-trivial component G_1. To prove the theorem, it is sufficient to show that G_1 contains a vertex with degree $|V(G_1)|-1$. This result holds when $m \le 2$. Next, we assume $m \ge 3$.

Choose a vertex $x \in G_1$ such that $d_x = \Delta$. If $d_x \le |V(G_1)|-2$, we can easily find two different vertices $y \in N(x)$ and $z \in N(y) - N(x) - x$. For convenience, let $A = N(x) - N(y) - y$, $B = N(x) \cap N(y)$, $C = N(y) - N(x) - x$ and $|C| = k \ge 1$. Note that A, B and C are pairwise disjoint. We construct a new graph G' from G by deleting yv and adding xv for all $v \in C$; see Figure 6. It is clear that $G' \in \mathcal{G}(n,m)$.

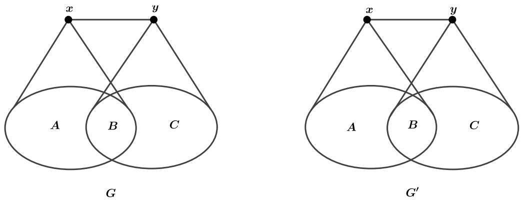

Figure 6. The graphs G and G' in the proof of Theorem 1.6.

Since $f(x,y)$ has the property P and satisfies that $f_1 > 0$ and $f_{11} > 0$, we have

$$\begin{aligned} TI_f(G') - TI_f(G) =& \sum_{v\in A\cup B\cup C} f(d_x+k, d_v) + \sum_{v\in B} f(d_y-k, d_v) + f(d_x+k, d_y-k) \\ &- \left[\sum_{v\in A\cup B} f(d_x, d_v) + \sum_{v\in B\cup C} f(d_y, d_v) + f(d_x, d_y)\right] \\ =& \sum_{v\in A}[f(d_x+k, d_v) - f(d_x, d_v)] + \sum_{v\in C}[f(d_x+k, d_v) - f(d_y, d_v)] \\ &+ \sum_{v\in B}[f(d_x+k, d_v) + f(d_y-k, d_v) - f(d_x, d_v) - f(d_y, d_v)] \\ &+ [f(d_x+k, d_y-k) - f(d_x, d_y)] > 0. \end{aligned}$$

Hence $TI_f(G') > TI_f(G)$, which contradicts the maximality of G.

The proof is thus complete. ■

Proof of Theorem 1.7: Noting that $d_u + d_v \le 1 + m$ for any $uv \in E(G)$, we have $f(d_u, d_v) \le f(d_u + d_v - 1, 1) \le f(m, 1)$. Thus

$$TI_f(G) = \sum_{uv \in E(G)} f(d_u, d_v) \le \sum_{e \in E(G)} f(1, m) \le mf(1, m),$$

with equality if and only if $G = K_{1,m} \cup (n - m - 1)K_1$. The proof is thus complete. ■

Proof of Theorem 1.8: Suppose G is a maximal graph in the family $\mathcal{G}^c(n, m)$ of connected graphs of order n and size m. Then by Theorem 1.6, we know that G has a universal vertex v. It follows from $m \ge n - 1$ that $d_x = n - 1$. Then we have

$$TI_f(G) = I_g(G - v) + H_h(G - v),$$

where $g(x, y) = f(x+1, y+1)$ and $h(x) = f(n-1, x+1)$. Notice that $|V(G-v)| = n-1$ and $|E(G - v)| = m - n + 1 = \gamma \le n - 2$.

First, we show that $g(x, y)$ and $G - v$ satisfy the conditions of Theorem 1.7. It is obvious that $g(x, y)$ is symmetric and $g_1 > 0$, since $g(x, y) = g(y, x)$ and $g_1(x, y) = f_1(x-1, y)$. For any four integers x_1, x_2, y_1 and y_2 satisfying the equation $x_1+y_1 = x_2+y_2$, $(x_1 - 1) + (y_1 - 1) = (x_2 - 1) + (y_2 - 1)$ is still a constant. Thus

$$g(x_1, y_1) = f(x_1 - 1, y_1 - 1) > f(x_2 - 1, y_2 - 1) = g(x_2, y_2)$$

if $|(x_1 - 1) - (y_1 - 1)| > |(x_2 - 1) - (y_2 - 1)|$, i.e., $|x_1 - y_1| > |x_2 - y_2|$. Applying Theorem 1.7, we have

$$I_g(G - v) \le \gamma g(\gamma, 1) = \gamma f(\gamma + 1, 2),$$

with equality if and only if $G - v$ is the union of a star and some isolated vertices.

To estimate $H_h(G-v)$, we apply Lemma 2.6. Since $h(x+1)-h(x) = f_1(n-1, x+1)$, $f_{11}(n - 1, x + 1) \ge 0$ implies that $h(x + 2) - h(x + 1) \ge h(x + 1) - h(x)$, which means that $h(x)$ is convex. Similarly, $f_{111}(n-1, x+1) \ge 0$ implies that $h_1(x) = h(x+1)-h(x)$ is convex. Consequently, we have

$$\begin{aligned} H_h(G - v) &\le h(\gamma) + \gamma h(1) + (n - \gamma - 2)h(0) \\ &= f(n - 1, \gamma + 1) + \gamma f(n - 1, 2) + (n - \gamma - 2)f(n - 1, 1). \end{aligned}$$

It implies that

$$
\begin{aligned}
TI_f(G) = I_g(G-v) + H_h(G-v) \leq \gamma f(\gamma+1,2) \\
+ f(n-1,\gamma+1) + \gamma f(n-1,2) + (n-\gamma-2) f(n-1,1),
\end{aligned}
$$

with equality if and only if $G - v$ is the union of a star and some isolated vertices, i.e., $G = K_1 \vee (K_{1,\gamma} \cup (n-\gamma-2)K_1)$.

The proof is now complete. ∎

Acknowledgement: The authors are grateful to the reviewers for their helpful comments and suggestions.

References

[1] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure–activity correlations, in: M. Charton, I. Motoc, *Steric Effects in Drug Design*, Springer–Verlag, Berlin, 1983, 21–55.

[2] B. Bollobás, P. Erdös, A. Sarkar, Extremal graphs for weights, *Discr. Math.* **200** (1999) 5–19.

[3] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[4] R. Cruz, J. Rada, The path and the star as extremal values of vertex–degree–based topological indices among trees, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 715–732.

[5] E. Estrada, The ABC matrix, *J. Math. Chem.* **55** (2017) 1021–1033.

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

[7] B. Furtula, I. Gutman, M. Dehmer, On structure–sensitivity of degree–based topological indices, *Appl. Math. Comput.* **219** (2013) 8973–8978.

[8] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

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

[10] Z. Hu, X. Li, D. Peng, Graphs with minimum vertex–degree function–index for convex functions, submitted to *MATCH Commun. Math. Comput. Chem.*

[11] X. Li, Z. Wang, Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree–based indices, *Lin. Alg. Appl.* **620** (2021) 61–75.

[12] J. Rada, R. Cruz, Vertex–degree–based topological indices over graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 603–616.

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

[14] I. Tomescu, Properties of connected (n, m)-graphs extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 285–294.

[15] I. Tomescu, Graphs with given cyclomatic number extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 109–114.

[16] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[17] Y. Yao, M. Liu, F. Belardo, C. Yang, Unified extremal results of topological indices and spectral invariants of graphs, *Discr. Appl. Math.* **271** (2019) 218–232.