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The F–Index for some Special Graphs and some Properties of the F–Index

ASGHAR YOUSEFI[1], ALI IRANMANESH[2,*], ANDREY A. DOBRYNIN[3] AND ABOLFAZL TEHRANIAN[1]

[1]Department of Mathematics, Science and Research Branch, Islamic Azad University, P. O. Box 14515 – 1775, Tehran, Iran
[2]Department of Mathematics, Tarbiat Modares University, P. O. Box 14115 – 137, Tehran, Iran
[3]Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk 630090, Russia

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ABSTRACT

The "forgotten topological index" or "F–index" has been introduced by Furtula and Gutman in 2015. The F–index of a (molecular) graph is defined as the sum of cubes of the vertex degrees of the graph. In this paper, we compute this topological index for some special graphs such as Wheel graph, Barbell graph and friendship graph. Moreover, the effects on the F–index are observed when some operations such as edge switching, edge moving and edge separating are applied to the graphs. Finally, we investigate degeneracy of F–index for small graphs.

1 INTRODUCTION

Throughout this paper, we only consider finite, connected, undirected and simple graphs. Let G be such a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $u \in V(G)$, $d_G(u)$ denotes the degree of u which is the number of edges incident to u and $N_G(u)$ is neighbor vertex set of u. Clearly $d_G(u) = |N_G(u)|$. The maximum degree of vertices in G is denoted by $\Delta(G)$. For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W together with their incident edges. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the

*Corresponding Author: (Email address:iranmanesh@modares.ac.ir)
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subgraph of G obtained by deleting the edges of E'. If $W = \{u\}$and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - u$ and $G - xy$ for short, respectively. For any two nonadjacent vertices x and y of graph G, we let $G + xy$ be the graph obtained from G by adding an edge xy. As usual, let C_n and K_n be the cycle and complete graph on n vertices, respectively.

Chemical graph theory is a branch of mathematical chemistry where molecular structures are modeled as molecular graphs. A molecular graph is a simple unweighted, undirected graph where the vertices correspond to the atoms in the molecule and the edges correspond to the covalent bonds between them. A single number, representing a chemical structure, in graph – theoretical terms, is called a *topological descriptor*. It must be a structural invariant, i.e., it does not depend on the labeling or the pictorial representation of a graph. If such a topological descriptor correlates with a molecular property, it is named *molecular index* or *topological index*. In fact, a topological index is numeric quantity derived from a molecular graph which correlates with the physico–chemical properties of the molecule. Different topological indices are used for quantitative structure–property relationship **(QSPR)** and quantitative structure–activity relationship **(QSAR)** [8,9,17,25].

In [15], Gutman and Trinajstić introduced the most famous vertex – degree based topological indices and named them as the *first Zagreb index* and *second Zagreb index*. These topological indices were elaborated in [14]. For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$of G are defined as follows:

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 \ \& M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

The first Zagreb index can also expressed as [10]:

$$M_1(G) = \sum_{uv\in E(G)}[d_G(u) + d_G(v)].$$

For more information on the Zagreb indices and their applications see [3, 4, 18, 24, 25, 28].

Gutman and Trinajstić in [15] obtained the approximate formulas for the total π–electron energy. In these formulas, there was the sum of the cubes of the degrees of all vertices of the molecular graph. This sum, except in a few works about the general first Zagreb index [20,21] and the zeroth – order general Randić index [16], has been completely neglected. Recently, Furtula and Gutman named this sum as "*forgotten topological index*" [11] and they studied some basic properties of this index. The forgotten topological index, or shortly the "*F–index*" $F(G)$ of a (molecular) graph G is defined as:

$$F(G) = \sum_{v\in V(G)} d_G(v)^3.$$

We can rewrite the F–index as [10]:

$$F(G) = \sum_{uv\in E(G)}[d_G(u)^2 + d_G(v)^2].$$

For more information on the F–index see [1, 2, 5, 6, 12, 13, 27].

In papers [2, 6, 12, 27], the authors computed the F–index for some special graphs and in papers [1,5,13], the authors presented some properties of the F–index. These motivate us to compute the F–index for some other special graphs and present some other properties of the F–index.

In this paper, we compute the F–index for some special graphs such as Wheel graph, Barbell graph and Friendship graph [23]. Moreover, the effects on this index are observed when some operations such as edge switching, edge moving and edge separating [22] are applied to the graphs. Finally, we investigate degeneracy the F–index for small graphs.

2. THE F–INDEX FOR SOME SPECIAL GRAPHS

2.1. WHEEL GRAPH

A Wheel graph is a graph with p vertices, formed by connecting a single vertex to all vertices of C_{p-1}. It is denoted as W_p [23]. Graphs W_4, W_5, W_6,W_7, W_8 and W_9 are shown in Figure 1.

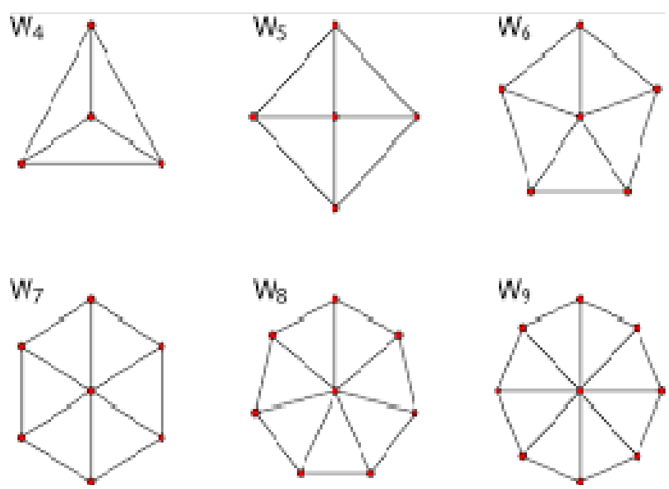

Figure 1. Graphs W_4, W_5, W_6,W_7, W_8 and W_9.

Wheel graphs are planar graphs and as such have a unique planar embedding. They are self–dual, the planar dual of any Wheel graph is an isometric graph. Any maximal planar graph, other than $K_4 = W_4$, contain as a subgraph either W_5 or W_6. There is always a Hamiltonian cycle in the Wheel graph and there are $(p^2 - 3p + 3)$ cycles in W_p [23].

Theorem 2.1. Let W_p be the Wheel graph with p vertices, $p \geq 4$, then its F–index is equal to $F(W_p) = (p-1)(p^2 - 2p + 28)$.

Proof. From the construction of Wheel graph W_p, it is clear that graph W_p has $p-1$ vertices with degree 3 and 1 vertex with degree $p-1$. Hence we have:

$$F(W_n) = \sum_{v \in V(W_p)} d_{W_p}(v)^3 = (p-1)(3)^3 + 1(p-1)^3$$
$$= (p-1)(p^2 - 2p + 28).$$

□

2.2. BARBELL GRAPH

A p–Barbell graph is the simple graph obtained by connecting two copies of a complete graph K_p by a bridge and it is denoted by B_p [23]. Graphs B_3, B_4, B_5 and B_6 are shown in Figure 2.

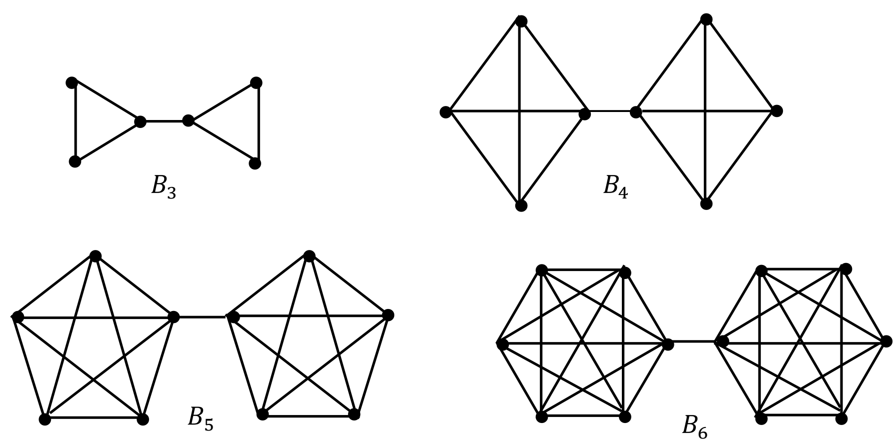

Figure 2. Graphs B_3, B_4, B_5 and B_6.

Theorem 2.2. Let B_p be the p – Barbell graph where $p \geq 3$, then its F–index is equal to $F(B_p) = 2[(p-1)^4 + p^3]$.

Proof. From the construction of graph B_p, it is clear that graph B_p has $2p-2$ vertices with degree $p-1$ and 2 vertices with degree p. Hence we have:

$$F(B_p) = \sum_{v \in V(B_p)} d_{B_p}(v)^3 = (2p-2)(p-1)^3 + 2p^3 = 2[(p-1)^4 + p^3].$$

□

2.3. Friendship Graph

A p – Friendship graph is the simple graph obtained by joining p copies of C_3 with a common vertex and it is denoted as F_p [23]. $F_p$is a planar undirected graph with $2p + 1$ vertices and $3p$ edges. Graphs F_2, F_3 and F_4 are shown in Figure 3.

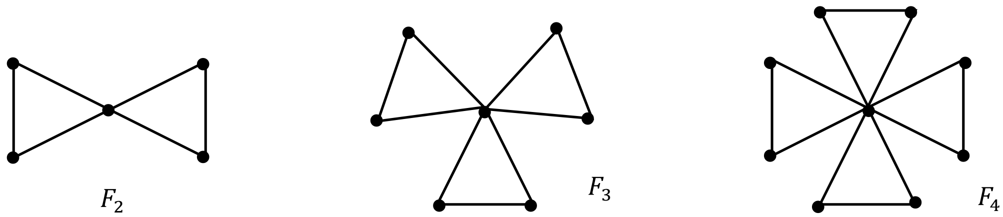

Figure 3. Graphs F_2, F_3 and F_4.

Theorem 2.3. Let F_p be the p–friendship graph, $p \geq 2$, then its F–index is equal to $F(F_p) = 8p(p^2 + 2)$.

Proof. From the construction of graph F_p, it is clear that graph F_p has $2p$ vertices with degree 2 and 1 vertex with degree $2p$. Hence we have:

$$F(F_p) = \sum_{v \in V(F_p)} d_{F_p}(v)^3 = 2p(2)^3 + 1(2p)^3 = 8p(p^2 + 2).$$

□

3. Some Properties of the F–Index

Proposition 3.1. Let G be a connected graph with two nonadjacent vertices $u, v \in V(G)$ and $G' = G + uv$. Then we have:

$$F(G') = F(G) + 2 + 3(d_G(u)^2 + d_G(u) + d_G(v)^2 + d_G(v)).$$

Proof. By the definition of the F–index, we have:

$$\begin{aligned} F(G') - F(G) &= (d_{G'}(u)^3 + d_{G'}(v)^3) - (d_G(u)^3 + d_G(v)^3) \\ &= (d_G(u) + 1)^3 - d_G(u)^3 + (d_G(v) + 1)^3 - d_G(v)^3 \\ &= 2 + 3(d_G(u)^2 + d_G(u) + d_G(v)^2 + d_G(v)), \end{aligned}$$

which completes the proof. □

From Proposition 3.1, we have the following corollary.

Corollary 3.1. If u and v are two nonadjacent vertices in graph G, then we have:

$$F(G + uv) > F(G).$$

3.1. EDGE SWITCHING OPERATION

Theorem 3.1.1. Let u and v be two nonadjacent vertices of a connected graph G with $d_G(u) \geq d_G(v)$. Suppose $v_1, v_2, \dots, v_s \in N_G(v) \setminus N_G(u), 1 \leq s \leq d_G(v)$. Let $G^* = G - \{vv_1, vv_2, \dots, vv_s\} + \{uv_1, uv_2, \dots, uv_s\}$, then $F(G^*) > F(G)$.

Proof. By the definition of the F–indexand the construction of graph G^*, we have:

$$\begin{aligned} F(G^*) - F(G) &= (d_{G^*}(u)^3 + d_{G^*}(v)^3) - (d_G(u)^3 + d_G(v)^3) \\ &= (d_G(u) + s)^3 - d_G(u)^3 + (d_G(v) - s)^3 - d_G(v)^3 \\ &= 3s(d_G(u)^2 - d_G(v)^2) + 3s^2(d_G(u) + d_G(v)) > 0. \end{aligned}$$

The last inequality follows from $d_G(u) \geq d_G(v)$. Therefore, $F(G^*) > F(G)$. □

Theorem 3.1.2. Let $\mathcal{G}_{n,m}$ be the set of connected graphs of order n and size m.Suppose $G \in \mathcal{G}_{n,m}$ with maximum F–index, then we have $\Delta(G) = n - 1$.

Proof. If $\Delta(G) = n - 1$, our result in this theorem holds immediately. If not, we choose a vertex u in the graph G with maximum degree and another vertex $v \in V(G)$ such that u is not adjacent to v. So we have $d_G(u) \geq d_G(v)$. Assume that $N_G(v) \setminus N_G(u) = \{v_1, v_2, \dots, v_s\}$. Note that $N_G(v) \setminus N_G(u) \neq \emptyset$ because of the fact that $d_G(u) < n - 1$. Now we construct a new graph G^* as:

$$G^* = G - \{vv_1, vv_2, \dots, vv_s\} + \{uv_1, uv_2, \dots, uv_s\}.$$

From Theorem 3.1.1, we have $F(G^*) > F(G)$. Thus we find that $G^* \in \mathcal{G}_{n,m}$ with a larger F–index than that of G. This is a contradiction to the choice of G, which finishes the proof of this theorem. □

3.2. EDGE MOVING OPERATION

Suppose v is a vertex of graph G. As shown in Figure 4. Let $G_{k,l}$ $(1 \leq k \leq l)$ be the graph obtained from G by attaching two new paths $P: v(= v_0)v_1v_2 \dots v_k$ and $Q: v(= u_0)u_1u_2 \dots u_l$ of length $k$and l, respectively, at v, where $v_1, v_2, \dots, v_k$ and $u_1, u_2, \dots, u_l$ are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$.

Theorem 3. 2. Let G be a connected graph of order $n \geq 2$ and $1 \leq k \leq l$**.**

(1) If $k \geq 2$, then $F(G_{k,l}) = F(G_{k-1,l+1})$.

(2) $F(G_{1,l}) > F(G_{0,l+1})$.

Proof (1). By the definition of the F–index and the construction of graph $G_{k,l}$, we have:

$$\begin{aligned}
F(G_{k,l}) - F(G_{k-1,l+1}) &= \left(d_{G_{k,l}}(v_{k-1})^3 + d_{G_{k,l}}(v_k)^3 + d_{G_{k,l}}(u_l)^3\right) \\
&\quad -\left(d_{G_{k-1,l+1}}(v_{k-1})^3 + d_{G_{k-1,l+1}}(u_l)^3 + d_{G_{k-1,l+1}}(v_k)^3\right) \\
&= (2^3 + 1^3 + 1^3) - (1^3 + 2^3 + 1^3) \\
&= 0,
\end{aligned}$$

which completes the Proof of (1).

Proof (2).

$$\begin{aligned}
F(G_{1,l}) - F(G_{0,l+1}) &= \left(d_{G_{1,l}}(v_1)^3 + d_{G_{1,l}}(v)^3 + d_{G_{1,l}}(u_l)^3\right) \\
&\quad -\left(d_{G_{0,l+1}}(v)^3 + d_{G_{0,l+1}}(u_l)^3 + d_{G_{0,l+1}}(v_1)^3\right) \\
&= \left(1^3 + \left(d_{G_{0,l+1}}(v) + 1\right)^3 + 1^3\right) \\
&\quad -\left(d_{G_{0,l+1}}(v)^3 + 2^3 + 1^3\right) \\
&= \left(3d_{G_{0,l+1}}(v)^2 + 3d_{G_{0,l+1}}(v) + 1^3 + 1^3\right) - (2^3) > 0\,.
\end{aligned}$$

Note that G is a connected graph with $n \geq 2$ vertices, so then $d_{G_{0,l+1}}(v) \geq 2$. Hence the last inequality follows easily. Therefore, $F(G_{1,l}) > F(G_{0,l+1})$. □

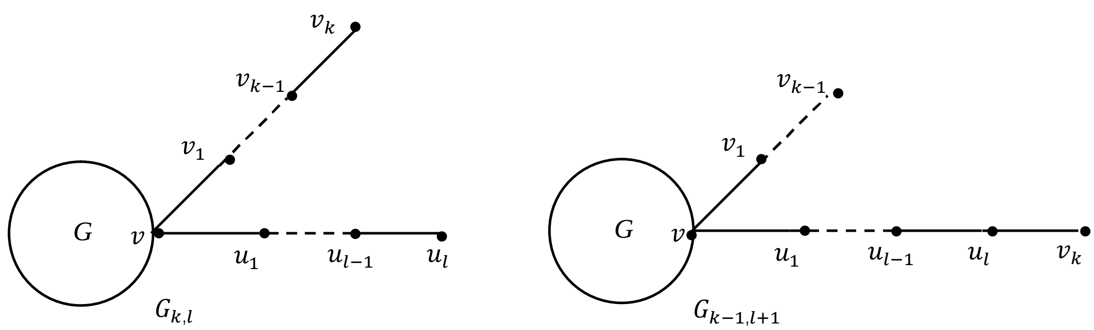

Figure 4.

3.3. EDGE SEPARATING OPERATION

Let $e = uv$ be a cut edge of a graph G. If G' is obtained from G by contracting the edge e into a new vertex u_e, which becomes adjacent to all the former neighbors of u and of v, and adding a new pendent edge $u_e v_e$, where v_e is a new pendent vertex. We say that G' is obtained from G by separating an edge uv (see Figure 5).

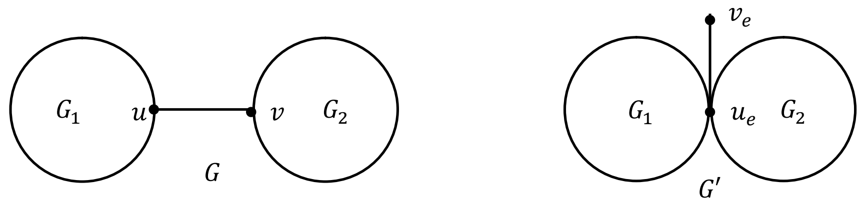

Figure 5.

Theorem 3.3. Let $e = uv$ be a cut edge of a connected graph G, where $d_G(u) \geq 2$ and $d_G(v) \geq 2$. Suppose G' is the graph obtained from G by separating the edge uv. Then $F(G') > F(G)$.

Proof: By the definition of the F–index and the construction of graph G', we have:

$$F(G') - F(G) = [d_{G'}(u_e)^3 + d_{G'}(v_e)^3] - [d_G(u)^3 + d_G(v)^3]$$
$$= [(d_G(u) + d_G(v) - 1)^3 + 1^3] - [d_G(u)^3 + d_G(v)^3]$$
$$-[d_G(u)^3 + d_G(v)^3]$$
$$= \left[\left(d_G(u) + d_G(v)\right)^3 - 3\left(d_G(u) + d_G(v)\right)^2 + 3\left(d_G(u) + d_G(v)\right)\right]$$
$$= 3(d_G(u) + d_G(v))(d_G(u)d_G(v) + 1) - 3\left(d_G(u) + d_G(v)\right)^2 > 0.$$

Since $d_G(u) \geq 2$and $d_G(v) \geq 2$, so then $d_G(u)d_G(v) \geq d_G(u) + d_G(v)$. Hence the last inequality follows easily. Therefore, $F(G') > F(G)$. □

3.4. k – APEX TREES

A tree is a connected acyclic graph. For any positive integer k with $k \geq 1$, a graph G is called a k – apex tree if there exists a subset X of $V(G)$ such that $G - X$ is a tree and $|X| = k$, while for any $Y \subseteq V(G)$ with $|Y| < k$, $G - Y$ is not a tree. A vertex of X is called a k – apex vertex [26]. For positive integers $n \geq 3$ and $k \geq 1$, let $\mathbb{T}(n, k)$ denote the class of all k – apex trees of orden n.

Theorem 3.4. Let $G \in \mathbb{T}(n, k)$ and v be a k – apex vertex of G. If $F(G)$ is maximum in $\mathbb{T}(n, k)$, then $d_G(v) = n - 1$.

Proof. Since $G \in \mathbb{T}(n, k)$, we have $|V(G)| = n$. Hence $d_G(u) \leq n - 1$ for all $u \in V(G)$. Suppose that $d_G(v) \neq n - 1$, so then $d_G(v) < n - 1$. Then there exists a vertex u in G such that $uv \notin E(G)$. Then by Corollary 3.1, we have $F(G +$

$uv) > F(G)$. Clearly $G + uv \in \mathbb{T}(n,k)$ and it contradicts to that $F(G)$ is maximum in $\mathbb{T}(n,k)$. Therefore, $d_G(v) = n - 1$. $\square$

Proposition 3.4. Let $G \in \mathbb{T}(n,k)$. If $F(G)$ is maximum in $\mathbb{T}(n,k)$, then we have:

$$|E(G)| = \frac{k(2n-k-3)}{2} + n - 1\,.$$

Proof. Let X be the set of all k – apex vertices in G. Then $|X| = k$. Since $F(G)$ is maximum in $\mathbb{T}(n,k)$, then by Theorem 3.4, we have $d_G(v) = n - 1$ for all $v \in X$ Hence the subgraph induced by X is a complete graph of order k and $G - X$ is a tree of order $n - k$. Thus

$$|E(G)| = \binom{k}{2} + k(n-k) + (n-k-1) = \frac{k(2n-k-3)}{2} + n - 1.$$

$\square$

3.5. Line Graph

The line graph, $L(G)$, of a graph G has the vertex set $V\big(L(G)\big) = E(G)$ and two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G share a common end vertex. The iterated line graph, $L^k(G)$, of G is defined as $L^k(G) = L(L^{k-1}(G))$, where $k \geq 1$ and $L^0(G) \cong G$. What we can say about values of the index with increasing k? We consider the case of r-regular graphs G, $r \geq 3$. Denote by r_k and n_k the degree and the order of $L^k(G)$, respectively. It is not hard to calculate that $r_k = 2^k(r-2) + 2$ and $n_k = \frac{1}{2^k} n \prod_{i=0}^{k-1} r_i$. Then $F(L^k(G)) = \frac{1}{2^k} n(2^k(r-2)+2)^3 \prod_{i=0}^{k-1}(2^i(r-2)+2)$. For example, the third line iteration of cubic graph G of order $n$gives $F\big(L^3(G)\big) = 9000n$.

4. Degeneracy the F–Index for Small Graphs

A topological index is called degenerate if it possesses the same value for more than one graph. A set of graphs with the same value of a given index forms a degeneracy class. Since a topological index can be regarded as a measure of structural similarity of molecular graphs, the finding of information on degeneracy classes can be useful for chemical applications. There are a number of functions for characterizing degeneration of topological indices [7]. The discriminating ability of an index for a family of graphs can be expressed by relation

{number of unique values of an index} / {number of the considered graphs}.

The number of unique values, of course, coincides with the number of degeneracy classes. The similar measure was introduced in [19] where the number of trivial degeneracy classes was used. Table 1 contains comparative data for trees, unicyclic and bicyclic graphs of small order. One can see that the discriminating ability of F-index is between discriminating ability of indices $M_1$and M_2.

n	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
	Trees																
M_1	1	1	.83	.64	.39	.28	.17	.09	.05	.03	.01	.006	.003	.001	.001	.000	.000
F	1	1	.83	.64	.49	.32	.19	.12	.08	.04	.02	.011	.006	.003	.001	.001	.000
M_2	1	1	1	.82	.74	.47	.33	.18	.10	.05	.03	.013	.007	.003	.001	.001	.000
	Unicyclic Graphs																
M_1	1	.8	.46	.27	.17	.07	.03	.014	.007	.003	.001	.001	.000	.000			
F	1	.8	.54	.33	.18	.01	.05	.024	.012	.006	.003	.001	.000	.000			
M_2	1	1	.77	.55	.30	.16	.08	.038	.017	.007	.003	.001	.001	.000			
	Bicyclic Graphs																
M_1	1	.6	.32	.15	.06	.024	.009	.004	.001	.000	.000						
F	1	.8	.47	.21	.09	.039	.017	.007	.003	.001	.000						
M_2	1	1	.74	.36	.16	.063	.025	.010	.004	.001	.000						

Table 1. Discriminating ability of indices for small n-vertex graphs.

Examples of trees of order 10, unicyclic graphs of order 11, and bicyclic graphs of order 13 for which these three indices coincide are presented in Figure 6. We have $F(T_1) = M_1(T_2) = M_2(T_3) = 66$, $F(G_1) = M_1(G_2) = M_2(G_3) = 88$, and $F(G_4) = M_1(G_5) = M_2(G_6) = 142$.

5. CONCLUSION

Topological indices are designed basically by transforming a molecular graph into a number. The "forgotten topological index" (F–index) was introduced recently by B. Furtula and I. Gutman in 2015 [11]. In this paper, we computed the F–index for some special graphs such as wheel graph, Barbell graph and Friendship graph. Moreover, the effects on the F–index were observed when some operations such as edge switching, edge moving and edge separating were applied to the graphs. However, there are still many other special graphs and operations which are not covered here. So, for further studies, F–index of some other special graph can be computed and also properties of the F–index under some other operations can be investigated.

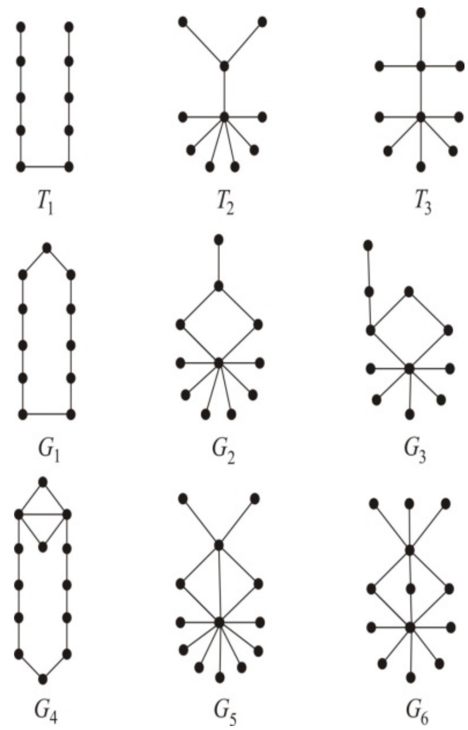

Figure 6. Graphs with the same indices.

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