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ONSOME NEW NEIGHBOURHOOD DEGREE BASED INDICES

Sourav Mondal[a], Nilanjan De[b*] and Anita Pal[a]

[a]*Department of Mathematics, National Institute of Technology, Durgapur, India.*

[b]*Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India.*

Abstract: In this paper, four novel topological indices named as neighbourhood version of forgotten topological index (F_N), modified neighbourhood version of Forgotten topological index ($F_N{}^*$), neighbourhood version of second Zagreb index ($M_2{}^*$) and neighbourhood version of hyper Zagreb index (HM_N) are introduced. Here the relatively study depends on the structure-property regression analysis is made to test and compute the chemical applicability of these indices for the prediction of physicochemical properties of octane isomers. Also it is shown that these newly presented indices have well degeneracy property in comparison with other degree based topological indices. Some mathematical properties of these indices are also discussed here.

Keywords:Topological indices, Zagreb index, Forgotten topological index, Neighbourhood Zagreb index.

Introduction

Throughout this article we use only molecular graph[1,2], a connected graph having no loops and parallel edges. In molecular graph nodes and edges

* N. De , *e-mail*: de.nilanjan@rediffmail.com

correspond to the atoms and chemical bonds of compound, respectively. Let G be a chemical graph containing $V(G)$and $E(G)$as vertex set and edge set respectively. The degree of a vertex v on a graph$G$, denoted by $deg_G(v)$, is the total number of edges associated with v. Let$N_G(v)$ denotes the set of neighbours of the vertex v. In chemical graph theory, topological indices play a leading role specifically in the quantitative structure property relationships and quantitative structure activity relationship modelling[3]. A topological index is a numeric value that is graph invariant. A real valued mapping considering graphs as arguments is called a graph invariant if it gives same value to isomorphic graphs. The order (total count of nodes) and size (total count of edges) of a graph are examples of two graph in variants. In chemical graph theory, the graph invariants are named as topological indices. The idea of topological indices was initiated when the eminent chemist Harold Wiener found the first topological index, known as Wiener index[4] in 1947 for searching boiling points of alkanes. One of the topological indices invented on initial stage is the so called Zagreb index first presented by Gutman and Trinajstić[5,6], where they investigated how the total energy of π-electron depends on the structure of molecules and it was discussed in details. The first $(M_1(G))$ and the second $(M_2(G))$ Zagreb indices for a molecular graph $G$are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} deg_G(v)^2 = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)],$$

$$M_2(G) = \sum_{uv \in E(G)} deg_G(u) deg_G(v).$$

For more discussion on these indices, inquisitive readers are referred the papers[7-16]. Furtula et al.[17] introduced the forgotten topological indices as follows:

$$F(G) = \sum_{v \in V(G)} deg_G(v)^3 = \sum_{uv \in E(G)} [deg_G(u)^2 + deg_G(v)^2].$$

For more discussion on this index readers are referred[18-20]. Following the first Zagreb index present authors[21] introduced a degree based topological index named as the Neighbourhood Zagreb index (M_N) which is defined as follows:

$$\delta_G(v) = \sum_{u \in N_G(v)} deg_G(u),$$

$$M_N(G) = \sum_{v \in V(G)} \delta_G(v)^2.$$

Inspiring from the Zagreb and Forgotten topological indices we present here four new topological indices named as neighbourhood version of forgotten topological index (F_N), modified neighbourhood version of Forgotten topological index ($F_N{}^*$), neighbourhood version of second Zagreb index ($M_2{}^*$) and neighbourhood version of hyper Zagreb index (HM_N)which are defined as follows:

$$F_N(G) = \sum_{v \in V(G)} \delta_G(v)^3,$$

$$F_N{}^*(G) = \sum_{uv \in E(G)} [\delta_G(u)^2 + \delta_G(v)^2],$$

$$M_2{}^*(G) = \sum_{uv \in E(G)} [\delta_G(u)\delta_G(v)],$$

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

The objective of this work is to discuss some mathematical properties and check the chemical applicability of these newly introduced indices. Here

we find the correlation coefficients of the newly designed indices and some well-established indices with acentric factor and entropy for octane isomers. In addition we investigate the degeneracy of the novel indices.

Preliminaries

In this section, we obtain some mathematical properties of the newly introduced indices. Applying some standard lemma, we compute some bounds of the aforesaid novel indices. We start with the following lemma:

Lemma 1. For a graph G, we have

(i) $\sum_{u \in V(G)}[\delta_G(u)] = M_1(G)$,

(ii) $\sum_{uv \in E(G)}[\delta_G(u) + \delta_G(v)] = 2M_2(G)$.

Lemma 2. (Cauchy-Schwartz inequality)[22]Let x_i and y_i be real numbers for all $1 \leq i \leq n$. Then

$$(\sum_{i=1}^{n} x_i y_i)^2 \leq (\sum_{i=1}^{n} {x_i}^2)(\sum_{i=1}^{n} {y_i}^2). \quad (1)$$

Equality holds $iff\ x_i = \mathrm{k}y_i$for some constant k and for each $1 \leq i \leq n$.

Proposition 1. Let G be a graph with m edges, whose second Zagreb index is $M_2(G)$, then we have

$$HM_N(G) \geq \frac{4M_2^2(G)}{m},$$

withequality holds $iff\ \delta_G(u) + \delta_G(v) = k$ for some constant k, $\forall uv \in E(G)$.

Proof. In (1), considering $x_i = \delta_G(u) + \delta_G(v), y_i = 1$, we have

$$\left(\sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)]\right)^2 \leq \sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)]^2 \sum_{uv \in E(G)} 1^2,$$

applying the definition of HM_N and lemma 1, we get the required result. From lemma 2, it is clear that equality holds $iff\ \delta_G(u) + \delta_G(v) = k$ for some constant k, $\forall uv \in E(G)$.

Lemma 3.[23]Let $(x_1, x_2, \dots, x_n)$ be positive n-tuple such that there exists positive number A, a satisfying $0 \leq a \leq x_i \leq A$, then we have

$$\frac{n\sum_{i=1}^{n} {x_i}^2}{\left(\sum_{i=1}^{n} x_i\right)^2} \leq \frac{1}{4}\left(\frac{\sqrt{A}}{\sqrt{a}} + \frac{\sqrt{a}}{\sqrt{A}}\right)^2, \tag{2}$$

where equality holds $iff\ a = A$ or $q = \frac{\frac{A}{a}}{\frac{A}{a}+1} n$ is an integer and q of the numbers x_i coincide with a and the remaining $(n-q)$ of the ${x_i}'$ s coincide with $A(\neq a)$.

For a graph G consider

$$\Delta_N = \max\{\delta_G(v): u \in V(G)\},$$
$$\delta_N = \min\{\delta_G(v): u \in V(G)\}.$$

Now putting $a = 2\delta_N,\ A = 2\Delta_N, x_i = \delta_G(u) + \Delta_G(v)$ in (2)and using lemma 1, we have the following proposition.

Proposition 2. Let G be a graph with m edges, whose second Zagreb index is $M_2(G)$, then we have

$$HM_N(G) \leq \frac{M_2(G)^2}{m}\frac{(\Delta_N + \delta_N)^2}{\Delta_N \delta_N},$$

where equality holds $iff\ \Delta_N = \delta_N$ or $q = \frac{\frac{\Delta_N}{\delta_N}}{\frac{\Delta_N}{\delta_N}+1} m$, is an integer and q of the numbers x_i coincide with δ_N and the remaining $(m-q)$ of the ${x_i}'$ s coincide with $\Delta_N(\neq \delta_N)$.

Lemma 4. Let $\vec{x} = (x_1, x_2, \dots, x_n)$ and $\vec{y} = (y_1, y_2, \dots, y_n)$ be sequence of real numbers. Also let $\vec{z} = (z_1, z_2, \dots, z_n)$ and $\vec{w} = (w_1, w_2, \dots, w_n)$be non-negative sequences. Then,

$$\sum_{i=1}^{n} w_i \sum_{i=1}^{n} z_i x_i^2 + \sum_{i=1}^{n} z_i \sum_{i=1}^{n} w_i y_i^2 \geq 2\sum_{i=1}^{n} z_i x_i \sum_{i=1}^{n} w_i y_i. \tag{3}$$

In particular, if z_i and w_i are positive, then the equality holds $iff\ \vec{x} = \vec{y} = \vec{k}$, where $\vec{k} = (k, k, \dots, k)$, a constant sequence.

Proposition 3. For any graph G with Neighbourhood Zagreb index and first Zagreb index $M_N(G)$ and $M_1(G)$ respectively, we have

$$F_N(G) \geq 2M_N(G) - M_1(G), \tag{4}$$

where equality holds $iff\ G$ is P_2.

Proof. Considering $x_i = \delta_G(u),\ y_i = 1,\ z_i = \delta_G(u), w_i = 1$ in (3), we obtain

$$\sum_{i=1}^{n} 1 \sum_{u\in V(G)} \delta_G(u)^3 + \sum_{u\in V(G)} \delta_G(u) \sum_{i=1}^{n} 1 \geq 2 \sum_{u\in V(G)} \delta_G(u)^2 \sum_{i=1}^{n} 1. \tag{5}$$

After using the definition of F_N and M_N indices and applying lemma 1, we obtain the required result. According to the lemma 3, the equality in (4) holds $iff\ \delta_G(u) = 1\ \forall\ u \in V(G), i.e.\ G$ is P_2. Hence the proof.

Lemma 5. (Radon's inequality) If $a_i, b_i > 0, i = 1,2, \dots, n, p > 0$, then

$$\frac{\sum_{i=1}^{n} a_i^{p+1}}{\sum_{i=1}^{n} b_i^{p}} \geq \frac{\left(\sum_{i=1}^{n} a_i\right)^{p+1}}{\left(\sum_{i=1}^{n} b_i\right)^{p}}, \tag{6}$$

where equality holds $iff\ a_i = kb_i$ for some constant $k, \forall i = 1,2, \dots, n$.

For a graph G, considering $a_i = \delta_G(u), b_i = 1, p = 2$, in (6), we have the following proposition.

Proposition 4. For any graph with *n* vertices, we have

$$F_N(G) \geq \frac{M_1(G)^3}{n}, \tag{7}$$

where equality holds $iff\ G$ is regular or complete bipartite graph.

Proposition 5. Let G be a graph, whose first and neighbourhood Zagreb indices are $M_1(G)$ and $M_N(G)$ respectively. Then

$$F_N(G) \geq \frac{M_N(G)^2}{M_1(G)}. \tag{8}$$

Proof. Let$G$ be a graph and $u \in V(G)$. The weighted averages of $\delta_G(u)$ and squares of $\delta_G(u)$ are

$$\langle d \rangle_w = \frac{\sum_{u\in V(G)} w(u)\delta_G(u)}{\sum_{u\in V(G)} w(u)},$$

$$\langle d^2 \rangle_w = \frac{\sum_{u \in V(G)} w(u) \delta_G(u)^2}{\sum_{u \in V(G)} w(u)},$$

where $w(u)$ is weight corresponding to the vertex u of G. For any non-negative weight, $\langle d^2 \rangle_w \geq (\langle d \rangle_w)^2$. Choosing $w(u) = \delta_G(u)$ and using definitions of $F_N(G)$, $M_N(G)$and $M_1(G)$,we obtain the bound (8).

Chemical significance of the newly introduced indices

According to the report of the IAMC (International Academy of Mathematical Chemistry), the chemical applicability of a topological index can be evaluated by regression analysis. Naturally 18 octane isomers are helpful for such investigation, since the number of the structural isomers of octane is large (18) enough to create the statistical perfection faithful. Furtulaet al.[17] shown that M_1 and F yield correlation coefficient greater than 0.95 with acentric factor and entropy for octane isomers. Also a simple linear model $(M_1 + \lambda F)$, where λ is varied from -20 to 20 is designed to improve the predictive ability of these indices. De et al.computed that the correlation coefficient of F-coindex for octane isomers in case of the logarithm of the octanol-water partition coefficient (P) is 0.966. In a recent work[24] the application possibilities of various graph irregularity indices for the prediction of physicochemical properties are described. We find the correlation of different physiochemical properties with $F_N, F_N{}^*, M_2{}^*$ and $HM_N$of octane isomers and good results are obtained in case acentric factor (Acent Fac.) and entropy (S) which are shown in this report (Table 2). The correlations of acentric factor and entropy with some well-known degree based topological indices are also investigated in Table 3. The results are also shown graphically in Figure 1 and Figure 2. The data of octane isomers (Table1) are collected fromwww.moleculardescriptors.eu/dataset/dataset.htm. Thus the newly

introduced indices can help to predict the entropy and acentric factor with powerful accuracy.

Table 1. Experimental values of the acentric factor, entropy (S) and the corresponding values of $F_N, {F_N}^*, {M_2}^*$,and HM_N.

Molecule name	**Acent Fac.**	**S**	$F_N(G)$	${F_N}^*(G)$	${M_2}^*(G)$	$HM_N(G)$
n-octane	0.397898	111.67	326	172	84	340
2-methyl heptane	0.377916	109.84	406	202	98	398
3-methyl heptane	0.371002	111.26	448	224	106	436
4-methyl heptane	0.371504	109.32	472	228	107	442
3-ethyl hexane	0.362472	109.43	520	252	115	482
2,2-dimethyl hexane	0.339426	103.42	632	282	132	538
2,3-dimethyl hexane	0.348247	108.02	582	282	129	540
2,4-dimethyl hexane	0.344223	106.98	558	258	121	500
2,5-dimethyl hexane	0.35683	105.72	486	232	113	458
3,3-dimethyl hexane	0.322596	104.74	728	324	148	620
3,4-dimethyl hexane	0.340345	106.59	630	306	136	578

Table 1. Continued

2-methyl-3-ethyl pentane	0.332433	106.06	666	312	137	586
3-methyl-3-ethyl pentane	0.306899	101.48	806	374	163	700
2,2,3-trimethyl pentane	0.300816	101.31	850	384	171	726
2,2,4-trimethyl pentane	0.30537	104.09	778	312	147	606
2,3,3-trimethyl pentane	0.293177	102.06	874	408	179	766
2,3,4-trimethyl pentane	0.317422	102.39	728	342	151	644
2,2,3,3-tetramethyl butane	0.255294	93.06	1070	488	217	922

Table 2. Correlation coefficient of $F_N, {F_N}^*, {M_2}^*$ and HM_N with acentric factor and entropy (S).

	$F_N(G)$	${F_N}^*(G)$	${M_2}^*(G)$	$HM_N(G)$
Acent Fac.	-0.99457	-0.97547	-0.98533	-0.98049
S	-0.93831	-0.93164	-0.94809	-0.93784

Table 3. Correlation coefficient of $M_1, M_2,$ and F with acentric factor and entropy (S).

	$M_1(G)$	$M_2(G)$	$F(G)$
Acent Fac.	-0.97306	-0.98642	-0.96505
S	-0.95429	-0.94169	-0.95272

Now, we depict the correlations discussed above in the following figures.

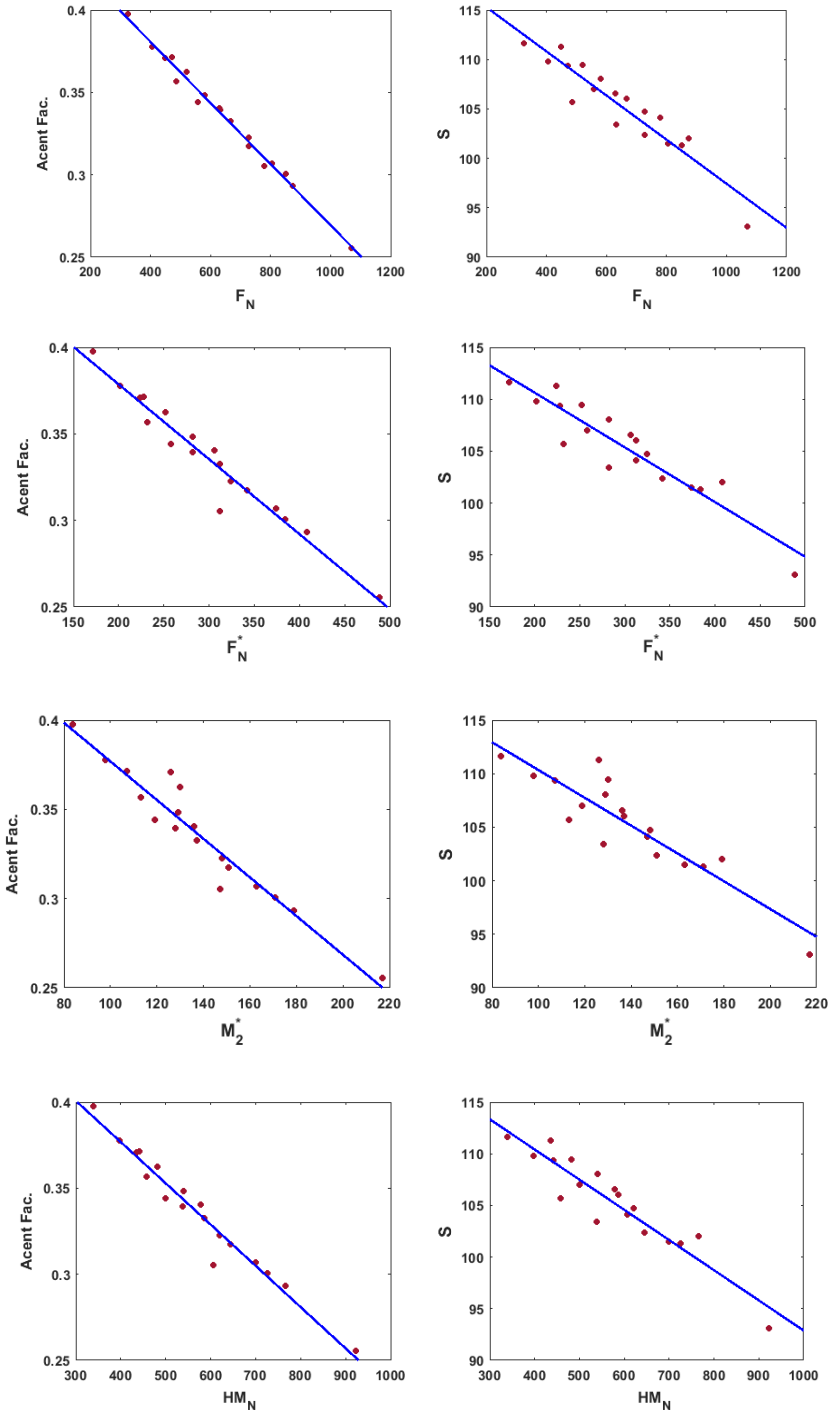


Figure 1. Correlations of acentric factor and entropy (*S*) with the newly introduced indices for octane isomers.

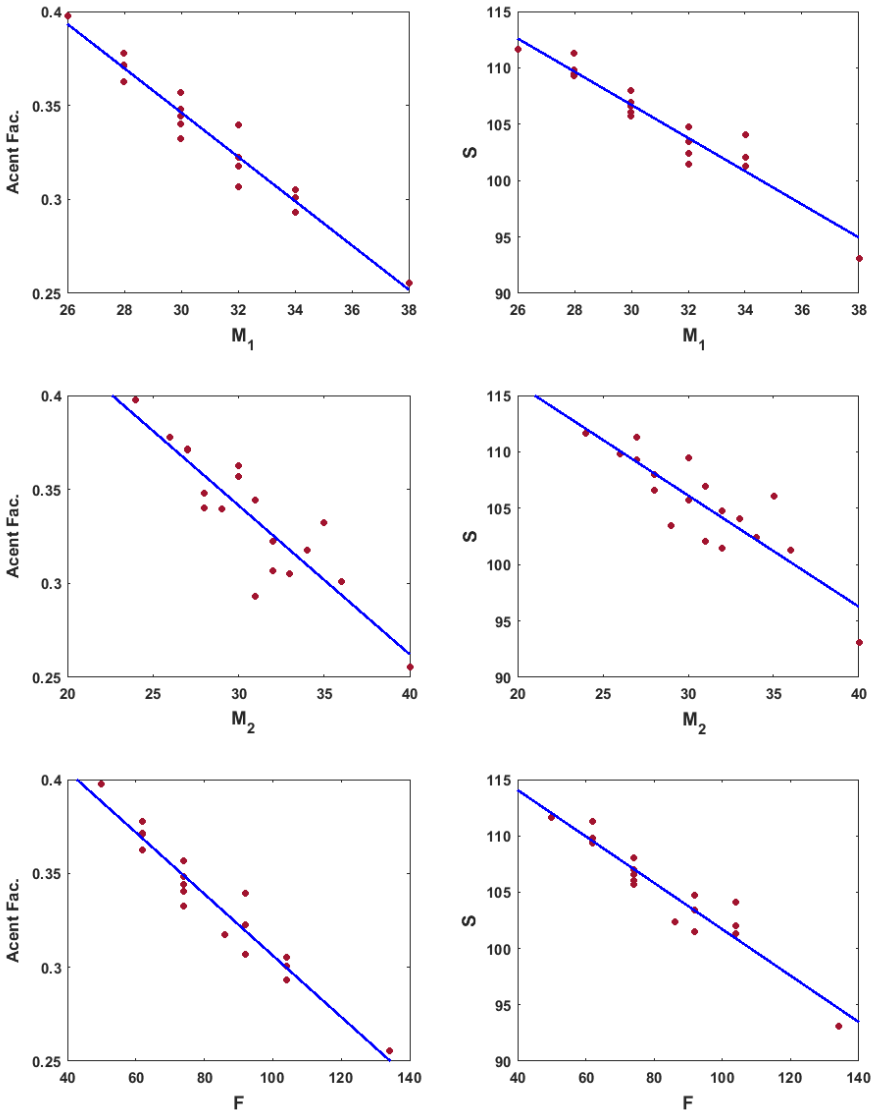


Figure 2. Correlations of acentric factor and entropy (S) with some well established indices (M_1, M_2, and F) for octane isomers.

The aim of molecular descriptors is to encode the structural characteristics of a molecule to the greatest extent possible. Ideally, a molecular descriptor should distinguish between two different structural formulae. A major drawback of most topological indices is their degeneracy,

i.e.,two or more isomers possess the same topological index. Topological indices having high discriminating power captures more structural information. We use the measure of degeneracy known as sensitivity introduced by Konstantinova[25], which is defined as follows:

$$S_I = \frac{N - N_I}{N},$$

where N is the total number of isomers considered and N_I is the number of them that cannot be distinguished by the topological index I. As S_I increases, the isomer-discrimination power of topological indices increases. The vertex degree based topological indices have more discriminating power in comparison with other classes of molecular descriptors. For octane isomers, the newly introduced indices exhibit good response among other investigated degree based indices (Table 4).

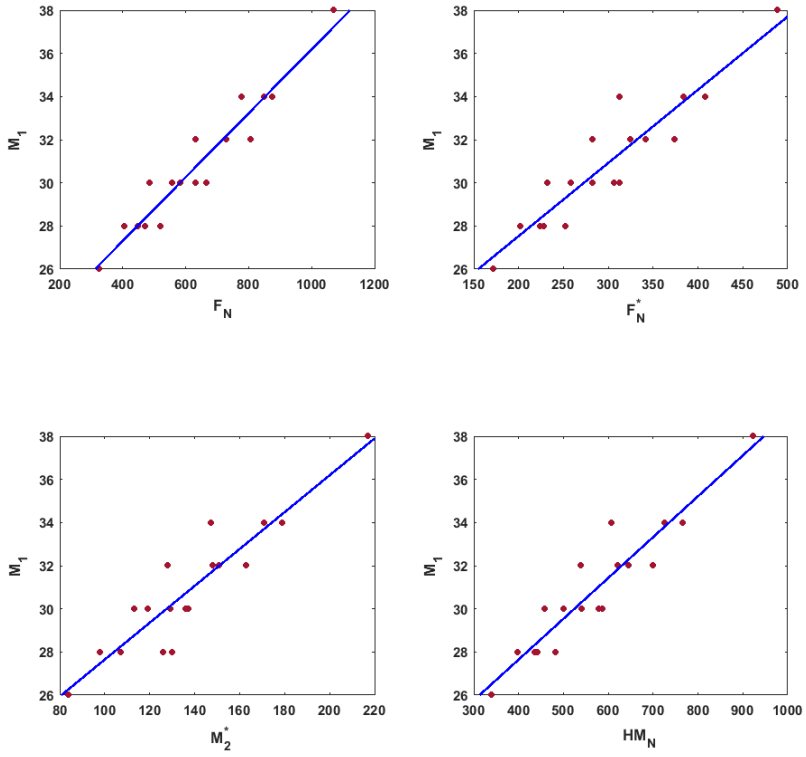
Table 4. Measure of sensitivity (S_I) of different indices for octane isomers.

Indices	**Sensitivity (S_I)**
M_2^*	**1.000**
HM_N	**1.000**
F_N	**0.944**
F_N^*	**0.889**
Connectivity index (χ)	0.889
Hyper Zagreb index(HM)	0.833
Second Zagreb index (M_2)	0.722
Hosoya index (Z)	0.778
Forgotten topological index (F)	0.389
First Zagreb index (M_1)	0.333

Also these new indices have very good correlations with some well-established degree based topological indices (Table 5) which can predict physiochemical properties with high accuracy. Thus we can say that these novel indices are chemically significant.

Table 5. Correlation coefficients of F_N, F_N^*, M_2^* and HM_N with some other indices.

	F_N	F_N^*,	M_2^*	HM_N	M_1	M_2	F
F_N	1						
F_N^*,	0.987	1					
M_2^*	0.992	0.996	1				
HM_N	0.989	0.999	0.999	1			
M_1	0.961	0.925	0.952	0.936	1		
M_2	0.991	0.997	0.998	0.998	0.948	1	
F	0.957	0.919	0.948	0.931	0.996	0.939	1



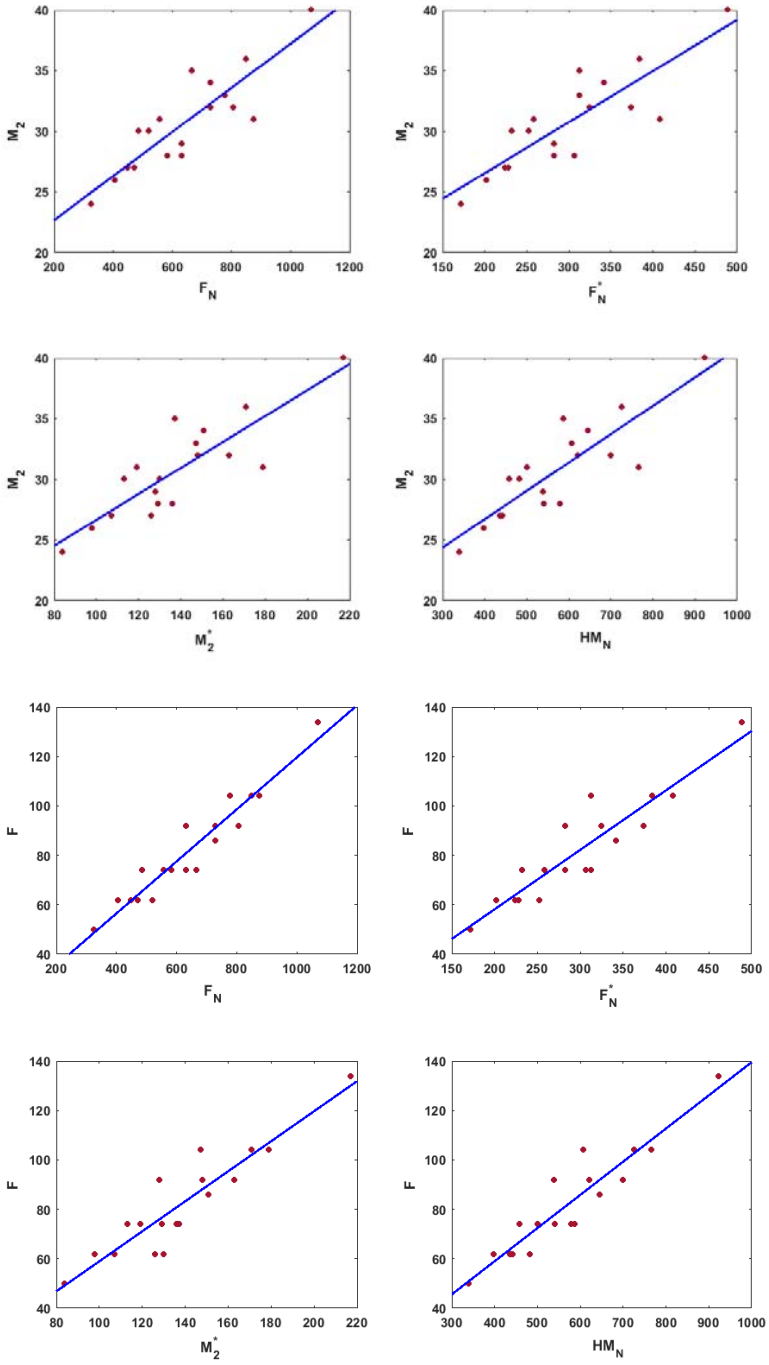


Figure 3. Correlations of some well-established degree based indices (M_1, M_2, and F) with novel indices.

Conclusion

In this report, we have introduced some new topological indices. Some mathematical properties of the newly proposed topological indices are discussed. Their chemical applicability is also investigated here. These indices have significant correlation with acentric factor and entropy in comparison with M_1, M_2 and F, shown in Table 2 and Table 3. Also Table 4 exhibits their supremacy in discriminative power in comparison to the other well-known investigated indices. Thus the four novel indices $F_N, {F_N}^*, {M_2}^*$ and HM_N deserve to be considered as applicable topological indices. We have correlated indices among themselves and with some other well-known degree-based topological indices in Table 5. From the correlations among the novel indices, it is clear that F_N and ${F_N}^*$ have good quality among four indices. For further research, these indices can be computed for various graph operations and some composite graphs and networks.

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References

1. Trinajesti´c, N. Chemical Graph Theory, *CRC Press, Boca Raton,* 1983.
2. Gutman, I.; Polansky, O.E. Mathematical Concepts in Organic Chemistry. *Springer, Berlin*, 1986.
3. Ashrafi, A.R.; Saheli, M.; Ghorbani, M. The eccentric connectivity index of nanotubes and nanotori. *J. Comput. Appl. Math.* **2011**, *235*, 4561-4566.
4. Das, K.C.; Xu, K.; Gutman, I. On Zagreb and Harary Indices. *MATCH Commun. Math. Comput. Chem.* **2013**, *70*, 301-314.
5. Gutman, I.; Trinajesti´c, N. Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535-538.
6. Gutman, I.; Ru´ci´c, B.; Trinajesti´c, N.; Wilcox, C.F. Graph theory and molecular orbitals. XII. Acyclic Polyenes. *J. Chem. Phys*. **1975**, *62*, 3399-3405.
7. Azari, M.; Iranmanesh, A. Chemical graphs constructed from rooted product and their Zagreb indices. *MATCH Commun. Math. Comput. Chem.* **2013**, *70*, 901-919.

8. Azari, M.; Iranmanesh, A.; Gutman, I. Zagreb indices of bridge and chain graphs. *MATCH Commun. Math. Comput. Chem.* **2013**, *70*, 921-938.

9. Fonseca, C.M.D.; Stevanovic, D. Further Properties of the Second Zagreb Index. *MATCH Commun. Math. Comput. Chem*. **2014**, *72*, 655-668.

10. Gutman, I.; Das, K.C. The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem*. **2004**, *50*, 83-92.

11. Hamzeh, A.; Reti, T. An analogue of Zagreb Index Inequality obtained from Graph irregularity measures. *MATCH Commun. Math. Comput. Chem*. **2014**, *72*, 669-683.

12. Li, S.; Zhang, M.J. Sharp bounds for the Zagreb indices of bipartite graphs with a given diameter. *Appl. Math. Lett.* **2011**, *24*, 131-137.

13. Ashrafi, A.R.; Doslic, T.; Hamzeh, A. The Zagreb coincides of graph operations. *Discret Appl. Math*. **2010**, *158*, 1571-1578.

14. De, N.; Nayeem, S.M.A.; Pal, A. The F-coindex of some graph operations. *Springer plus.* **2016**, *5*, article 221.

15. Das, K.C. On geometrical-arithmetic index of graphs. *MATCH Commun. Math. Comput. Chem*. **2010**, *64*, 619-630.

16. Ghorbani, M; Hosseinzadeh, M.A. The third version of Zagreb index. *Discret. Math. Algorithm. Appl.* **2013**, *5*, article 1350039.

17. Furtula, B.; Gutman, I. Forgotten topological index. *J. Math. Chem*. **2015**, *53*, 1184-1190.

18. De, N.; Nayeem, S.M.A.; Pal, A. F-index of some graph operations. *Discret. Math. Algorithm. Appl.* **2016**, *8*, article 1650025.

19. Che, Z.; Chen, Z. Lower and upper bounds of the Forgotten topological index. *MATCH Commun. Math. Comput. Chem*. **2016**, *76*, 635-648.

20. Akhtera, S; Imran, M. Computing the forgotten topological index of four operations on graphs. *AKCE Int. J. Graphs Comb.* **2017**, *14*, 70-79.

21. Mondal, S.; De, N.; Pal, A. On Neighbourhood Zagreb index of product graphs. *J. Taibah Univ. Sci.* (submitted).

22. Hardy, G.H.; Littlewood, J.E.; Polya, G. Inequalities, *Cambridge Univ Press*, 1988.

23. Polya, G.; Szego, G. Problems and theorems in analysis, in: Series, Integral Calculas, Theory of Functions, *Springer-Verlag*, vol. I, 1972.

24. Reti, T.; Sharafdini, R.; Dregelyi-Kiss, A.; Haghbin, H. Graph irregularity indices used as molecular descriptors in QSPR studies. *MATCH Commun. Math. Comput. Chem*. **2018**, *79*, 509-524.

25. Konstantinova, E.V. The Discrimination Ability of Some Topological and Information Distance Indices for Graphs of Unbranched Hexagonal Systems. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 54-57.