Reverse eccentric connectivity index

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Research on the topological indices based on eccentricity of vertices of a molecular graph has been intensively rising recently. Eccentric connectivity index, one of the best-known topological index in chemical graph theory, is belonging to this class of indices. In this paper, we introduce a novel topological index based on the eccentricity of vertices and its basic features are presented here. We named it as *reverse eccentric connectivity index*(*REEC)*.

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1. Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. There are numerous of topological descriptors that have found some applications in therotical chemistry, especially in QSPR/QSAR research. The eccentric connectivity index of the molecular graph *G*, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [2]. It is defined as;

$$ECC(G) = \xi^c(G) = \sum_{v \in V(G)} d(v).\varepsilon(v),$$

where $d(v)$ denotes the degree of the vertex *v* in *G* and $\varepsilon(v) = \max\{d(u,v) \mid u \in V(G)\}$ denotes the eccentricity of the vertex *v*. The eccentric connectivity index has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [3-10]. Recently a number of papers have appeared about mathematical properties of this topological index (for example see [11,12] and references cited therein). Recently, a novel graph invariant for predicting biological and physical properties – eccentric distance sum was introduced by Gupta, Singh and Madan [13]. It has a vast potential in structure activity/property relationships. The authors [13] have shown that some structure activity and quantitative structure-property studies using eccentric distance sum were better than the corresponding values obtained using the Wiener index [14], defined as;

$$W(G) = \sum_{v \in V(G)} D(v),$$

where $D(v)$ denotes the sum of all distances from v. The eccentric distance sum of *G* (*EDS*) is defined as;

$$\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) D(v).$$

For mathematical properties of this topological index see [15,16].

Here, we are proposing a new index which belonging to this class of topological
indices. It is defined as follows:

$$REEC(G) = {}^{RE}\xi^c = \sum_{v \in V(G)} \frac{\varepsilon(v)}{S(v)}$$

where summation goes over all vertices of graph *G*, $\varepsilon(v)$ denotes the eccentricity of the vertex *v* and $S(v)$ is the sum of degrees of all vertices adjacent to vertex *v*. This index is named as *reverse eccentric connectivity index (REEC),* ${}^{RE}\xi^c$. In the following sections, predictive power of *REEC* index will be discussed as well as its some basic mathematical properties.

2. Reverse eccentric connectivity index as possible tool for QSPR/QSAR research

In order to investigate predictive power of reverse eccentric connectivity index ${}^{RE}\xi^c$ we used octanes and some of their physico-chemical properties as resource. We found experimental results at the www.moleculardescriptors.eu. The following physico-chemical properties have been modeled:

- Entropy (*S*)
- Enthalpy of vaporization (*HVAP*)
- Standard enthalpy of vaporization (*DHVAP*)
- Acentric factor (*AcenFac*)

and results are compared with those obtained using the well-known Eccentric connectivity index. We chose those physico-chemical properties for which Reverse eccentric connectivity index (REEC) and Eccentric connectivity index (ECC) give reasonably good correlations, i.e. correlation coefficients are larger than 0.88. In the Table 1 are depicted graphs that show correlations between Reverse eccentric connectivity index (REEC) and Eccentric connectivity index (ECC) on one hand and above-mentioned properties on the other. From depicted graphs, it is not obvious which index gives better results.

Therefore, we conducted a simple statistical analysis to compare Reverse eccentric connectivity index (REEC) and Eccentric connectivity index(ECC) . Results are presented in Table 2.

Table 1. Graphs showing correlation between some phyisico-chemical properties and Reverse eccentric connectivity index (REEC) and Eccentric connectivity index (ECC) respectively.

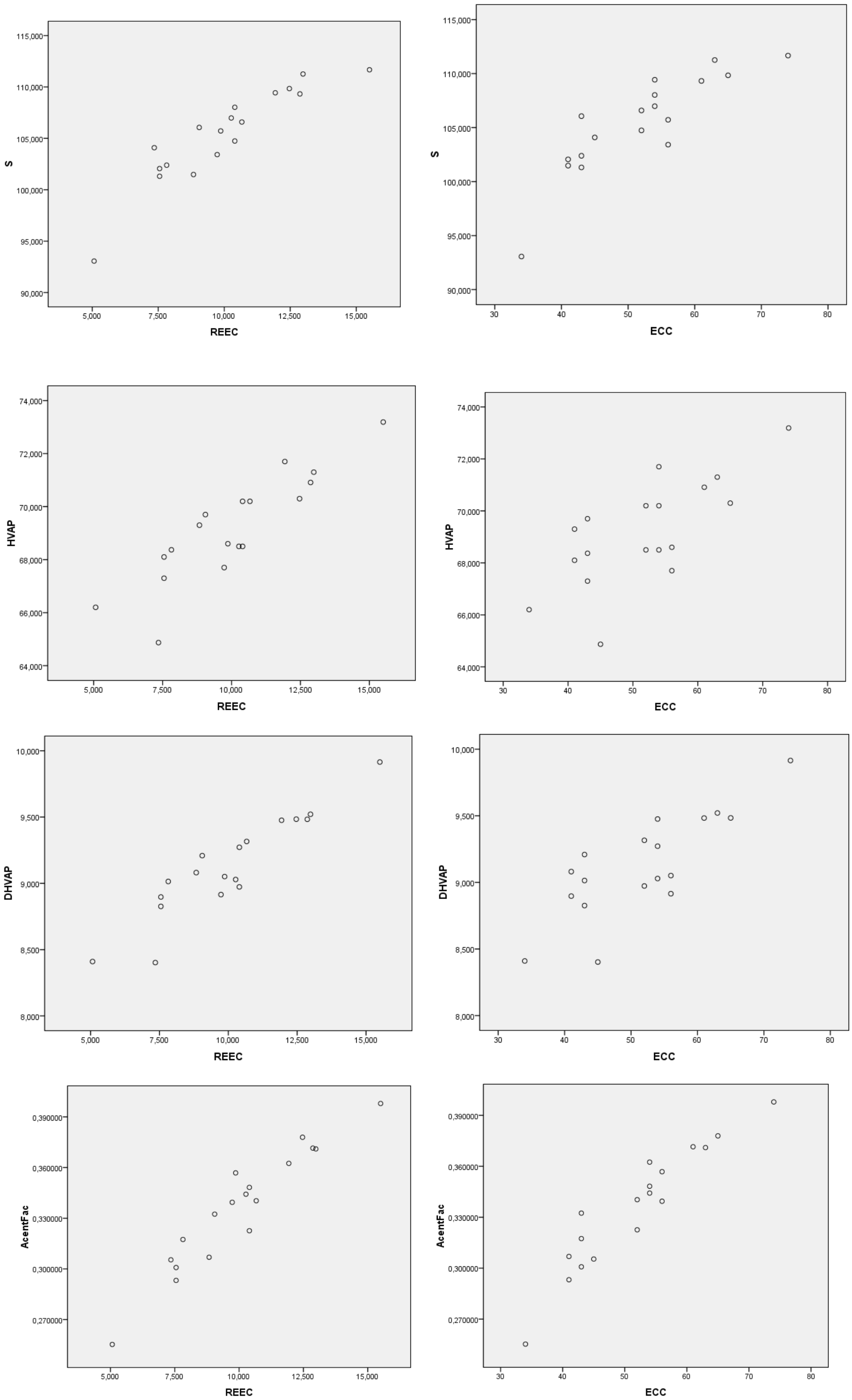

Table 2. Correlation coefficients and ratio of quadratic mean of residuals for graphs depicted in Table 1.

	Correlation coefficient (*R*)		*1-RQR(%)*
	REEC index	*ECC* index	
Entropy (*S*)	0,915	0,864	10,7
Enthalpy of vaporization (*HVAP*)	0,880	0,723	10,1
Standard enthalpy of vaporization (*DHVAP*)	0,925	0,803	10,8
Acentric factor (*AcenFac*)	0,953	0,943	10,2

It can be seen from data for correlation coefficient (R) (Table2) that in all cases Reverse eccentric connectivity index gives somewhat better results. Apparently, a superficial glance on the correlation coefficients do not show strong justification for introducing a new index, because correlation coefficients that we obtain in the case of Reverse eccentric connectivity index are not significantly better than those obtained using Eccentric connectivity index. However, predicting power of a new index is reasonable and that can be seen from the ratio of quadratic mean of residuals (RQR):

$$RQR = \frac{\sqrt{\frac{\sum_{i=1}^{n}(a.REEC_i + b - Exp_i)^2}{n}}}{\sqrt{\frac{\sum_{i=1}^{n}(a^{'}.ECC_i + b^{'} - Exp_i)^2}{n}}} = \sqrt{\frac{\sum_{i=1}^{n}(a.REEC_i + b - Exp_i)^2}{\sum_{i=1}^{n}(a^{'}.ECC_i + b^{'} - Exp_i)^2}}$$

One should observe that in all cases, the prediction power of Reverse eccentric connectivity index is at least for 10.1% better than prediction power of Eccentric connectivity index. The greatest improvement in prediction with Reverse eccentric connectivity index comparing to Eccentric connectivity index is obtained in the case of standard enthalpy of vaporization (10.8%). That is why we believe that Reverse eccentric connectivity index (REEC) should be considered in the future QSPR/QSAR researches.

3. Lower and upper bounds of Reverse eccentric connectivity index for general graphs and chemical graphs

In this section are given some basic mathematical features of Reverse eccentric connectivity index. For special classes of graphs we compute the following useful values for our parameter, using from definition.

$$^{RE}\xi^{c}(K_n) = \frac{n}{(n-1)^2}.$$

$$^{RE}\xi^{c}(K_{m,n}) = \frac{2(m+n)}{m.n}.$$

For the star, cycle and path of order *n*,

$$^{RE}\xi^{c}(S_n) = 2 + \frac{1}{n-1}.$$

$$^{RE}\xi^{c}(C_n) = \frac{n.\lfloor n/2 \rfloor}{4}.$$

$$^{RE}\xi^{c}(P_n) = \begin{cases} \frac{9n^2+26n-43}{48}, & \text{for } n \text{ is } odd(n \geq 5). \\ \frac{9n^2+26n-40}{48} & \text{for } n \text{ is } even(n \geq 4). \end{cases}$$

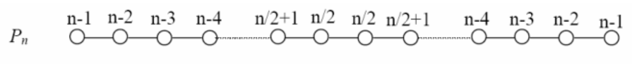

Fig. 1. The graphs P_n and its vertices' eccentricities when n is even.

Theorem 1 *Let G be a simple connected graph with n* $(n \geq 4)$ vertices, then

$$\frac{n}{(n-1)^2} \leq REEC(G) \leq \frac{9n^2+26n-40}{48}.$$

Lower bound is achieved if and only if G is an complete graph and upper bound is achieved if and only if G is a path.

Proof It is obvius that the only graph with its diameter *d=1* and the sum $S(v)$ equals its maximum is a complete graph. We can directly write from the definition of the *Reverse eccentric connectivity index* for *n* vertex complete graph K_n in which its vertex set is $V = \{1, 2, ..., n\}$;

$$^{RE}\xi^{c}(K_n) = \sum_{v \in K_n} \frac{\varepsilon(v)}{S(v)} = \frac{1}{(n-1)^2} + ... + \frac{1}{(n-1)^2} = \frac{n}{(n-1)^2}.$$

Again the only graph with *n* vertices has maximum eccentricity or diameter *n-1* and the sum $S(v)$ equals its minimum is a path. For *n* is even from the definiton we can write;

$$^{RE}\xi^{c}(P_n) = 2\left(\frac{n-1}{2} + \frac{n-2}{3} + \frac{n-3}{4} + \frac{n-4}{4} + ... + \frac{n/2}{4}\right) = \frac{9n^2+26n-40}{48}$$

And this completes the proof (See Fig. 1). If *n* is odd the proof made similarly.

Theorem 2 *Let T be a tree with n* $\left(n \geq 4\right)$ *vertices, then*

$$2+\frac{1}{n-1} \leq REEC(T) \leq \frac{9n^2+26n-40}{48}.$$

Lower bound is achieved if and only if T is a star and upper bound is achieved if and only if T is a path.

Proof The upper bound follows from Theorem 1. Let us prove the lower bound. Notice that the only tree with the minimum eccentricity and the minimum sum $S(v)$ is a star. Obviously for the central vertex *v* of any star $\varepsilon(v)=1$, $S(v)=n-1$ and for other vertices *u*, $\varepsilon(u)=2$, $S(u)=n-1$. We can directly write from the definition of the *Reverse eccentric connectivity index* for *n* vertex star graph S_n in which its vertex set is $V=\{1,2,...,n\}$;

$^{RE}\xi^c(S_n)=\sum_{v\in K_n}\frac{\varepsilon(v)}{S(v)}=\frac{1}{n-1}+\left(n-1\right).\frac{2}{\left(n-1\right)}=2+\frac{1}{n-1}$ It is clear that Theorem 2 holds for chemical trees.

Theorem 3 *Let* $G=(V,E)$ *be a connected graph of order n, minimum degre* δ *and diameter d . Then* , $^{RE}\xi^c(G)<\frac{n.d}{\delta}$.

Proof Let the vertex set is $V(G)=\{1,2,...,n\}$. From the definition of the *Reverse eccentric connectivity index* can be written for any connected graph *G*,

$$^{RE}\xi^c(G)=\sum_{i=1}^{n}\frac{\varepsilon(i)}{S(i)}=\frac{\varepsilon(1)}{S(1)}+\frac{\varepsilon(2)}{S(2)}+...+\frac{\varepsilon(n)}{S(n)}$$
$$<\frac{d}{\delta}+\frac{d}{\delta}+...+\frac{d}{\delta}=\frac{n.d}{\delta}.$$

Theorem 4 *Let* $G=(V,E)$ *be a k-regular graph of order n, radius r and diameter d . Then,* $\frac{n.r}{k^2} \leq {}^{RE}\xi^c(G) \leq \frac{n.d}{k^2}$ *with equality from the both side if and only if G is a complete graph.*

Proof Since the every vertex of *V(G)* adjacent to exactly *k* vertex and for any neighbouring vertex $S(v)=k^2$, the desired result is acquired from the definiton.

4. Conclusion

We proposed a new topological index based on eccentricity of vertices. It has been shown that this index can be used as predictive tool in QSPR/QSAR researches. Predictive power of this index has been tested on some physico-chemical properties of octanes. Obtained results show that it gives better results comparing with well-known Eccentric connectivity index. In addition, we analyzed some of its basic mathematical properties. It has been found a lower and upper bounds in the case of simple connected graphs and trees as well as in the case of chemical graphs and chemical trees. We also give lower and upper bounds for the Reverse eccentric connectivity index of connected graphs in terms of graph invariants such as the number of vertices (*n*), the radius (*r*) , the diameter (*d*) and the minimum degree (δ).

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