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On Variable Zagreb Indices*

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A novel variant of the Zagreb indices introduced in 1972, called the variable Zagreb indices, is presented. Their performance in the QSPR modeling of lower (C_3–C_8) alkane boiling points is compared with the original Zagreb indices and their modifications. The variable Zagreb indices produce better single-descriptor models and participate in better two- and three-descriptor models.

INTRODUCTION

The Zagreb M_1 and M_2 indices were introduced[1] and applied to the branching problem[2] in the early seventies of the last century when only the Wiener index[3] and the Hosoya *Z*-index[4] were known and used in QSPR.[5,6] Thirty years later there is still interest in Zagreb indices[7] and consequently the overall Zagreb indices[8] and their modified forms[9] are proposed and used.

The Zagreb indices and their variants have been used to study molecular complexity[10–14] and chirality[15] whilst the overall Zagreb indices[8] exhibit a potential applicability for deriving multilinear regression models. Various researchers also use the Zagreb indices in their QSPR and QSAR studies.[5–8,15,16–24] Mathematical properties of the Zagreb indices were also subjects of several studies.[25–27] These indices are referred to in most books reporting topological indices and their uses in QSPR and QSAR,[5–7,28] and they are also included in a number of programs used for the routine computation of topological indices, *e.g.* Refs. 29–32.

Here we report a further development of the Zagreb indices, the so-called variable Zagreb indices.

DEFINITION OF ORIGINAL ZAGREB INDICES

The original Zagreb indices are defined as follows:[1,2]

$$M_1 = \sum_{\text{vertices}} d(i)\, d(i) \tag{1}$$

$$M_2 = \sum_{\text{edges}} d(i)\, d(j) \tag{2}$$

where $d(i)$ is the degree of vertex i and $d(i)\ d(j)$ is the weight of edges i-j.

DEFINITION OF MODIFIED ZAGREB INDICES

A problem with the Zagreb indices, like with many other topological indices, is that their contributing parts give greater weights to the inner (interior) vertices and edges than to the outer (terminal) vertices and edges of a graph, as it can be seen from Figure 1.

This opposes intuitive reasoning that the outer atoms and bonds should have greater weights than the inner atoms and bonds because the outer atoms and bonds are associated with the larger part of the molecular surface and

* Dedicated to Professor Nenad Trinajstić, who is our scientific father, on the occasion of his 65th birthday.

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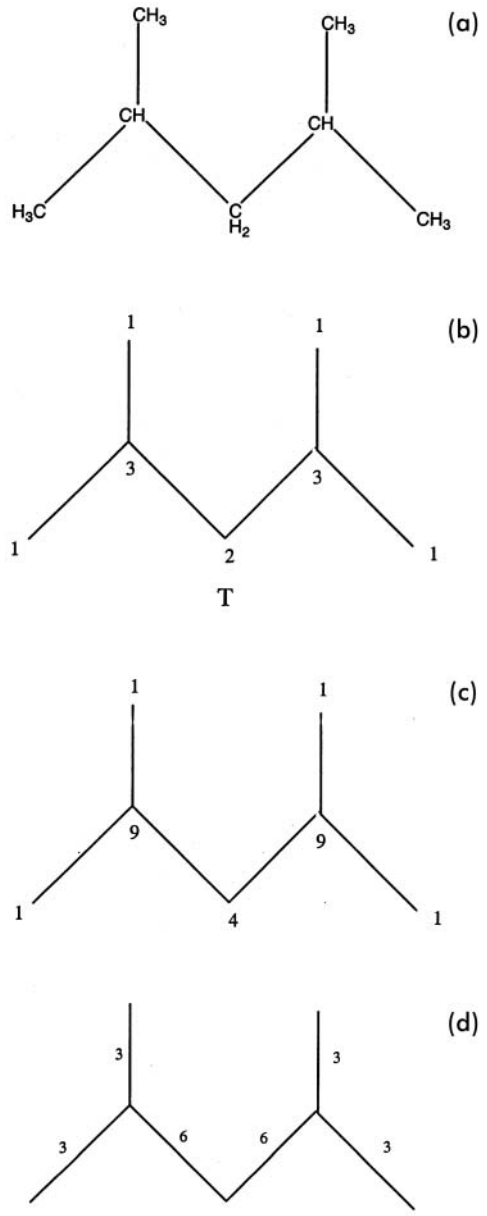

Figure 1. Contributing weights to the M_1 and M_2 indices of 2,4-dimethylpentane. (a) 2,4-dimethylpentane. (b) Hydrogen-suppressed tree T corresponding to 2,4-dimethylpentane and the vertex-degrees. (c) Vertex-weights contributing to the M_1 index of T. (d) Edge-weights contributing to the M_2 index of T.

are consequently expected to make a greater contribution to physical, chemical and biological properties.

Nikolić *et al.*[9] amended the Zagreb indices by putting inverse values of the vertex-degrees into Eqs. (1) and (2). These indices were named the modified Zagreb indices and were denoted by ${}^{m}M_1$ and ${}^{m}M_2$. They are given below:

$$ {}^{m}M_1 = \sum_{\text{vertices}} 1/[d(i)\, d(i)] = \sum_{\text{vertices}} [d(i)\, d(i)]^{-1} \qquad (3) $$

$$ {}^{m}M_2 = \sum_{\text{edges}} 1/[d(i)\, d(j)] = \sum_{\text{edges}} [d(i)\, d(j)]^{-1} \qquad (4) $$

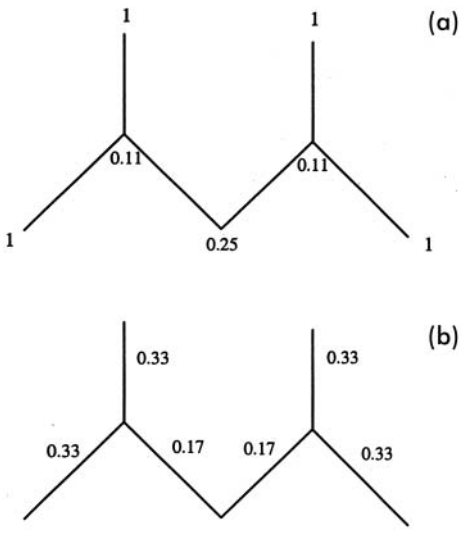

Figure 2. Contributing weights to the ${}^{m}M_1$ and ${}^{m}M_2$ indices of 2,4-dimethylpentane. (a) Vertex-weights contributing to the ${}^{m}M_1$ index of T. (b) Edge-weights contributing to the ${}^{m}M_2$ index of T.

Values ${}^{m}M_1$ and ${}^{m}M_2$ for the 2,4-dimethylpentane tree are given in Figure 2.

Comparing M_1 and M_2 indices with ${}^{m}M_1$ and ${}^{m}M_2$ for the 2,4-dimethylpentane tree we can see that modified Zagreb indices give greater weights to the outer vertices and edges than to the inner vertices and edges in accordance with the chemist's intuition.

VARIABLE ZAGREB INDICES

Eqs. (1) and (3) and Eqs. (2) and (4) can be collectively expressed as:

$$ {}^{v}M_1 = \sum_{\text{vertices}} [d(i)\, d(i)]^{\lambda} \qquad (5) $$

$$ {}^{v}M_2 = \sum_{\text{edges}} [d(i)\, d(j)]^{\lambda} \qquad (6) $$

where ${}^{v}M_1$ and ${}^{v}M_2$ denote variable Zagreb M_1 and M_2 indices. Obviously, for $\lambda = 1$ Eq. (5) reduces to Eq. (1) and Eq. (6) to Eq. (2), and for $\lambda = -1$ Eq. (5) reduces to Eq. (3) and Eq. (6) to Eq. (4). In this work we searched for the optimal value of λ. In order to determine λ, we used the set of C_3–C_8 alkanes and their boiling points. This set of alkanes was selected because a number of papers report the modeling of their boiling points.[9,33–35]

We considered the following a single-descriptor structure-boiling point relationship:

$$ \text{bp} = a + b\ \text{TI} \qquad (7) $$

where bp stands for the boiling point and TI (topological index) for the variable Zagreb indices ${}^{v}M_1$ and ${}^{v}M_2$.

We also considered the two-descriptor relationship:

$$\mathrm{bp} = a + b\ \mathrm{TI} + c\ \mathrm{TI'} \qquad (8)$$

where TI' was either p_3 or *twc*. p_3 is the polarity index[3], which is equal to the number of paths of length 3 and encodes the steric aspects of an alkane.[36] *twc* is the total walk count[34] and is shown to be a very useful descriptor in building multivariate QSPR models.

Finally, we tested the three-descriptor relationship:

$$\mathrm{bp} = a + b\ \mathrm{TI} + c\ p_3 + d\ twc \qquad (9)$$

We varied the exponent for ${}^{\mathrm{v}}M_1$ and ${}^{\mathrm{v}}M_2$ from $\lambda = 1$ to $\lambda = -1$ in order to detect that values of λ for which the variable Zagreb indices give the structure-boiling point models with the lowest value of the standard error of estimate s and the highest value of the correlation coefficient R. This is the origin of the term variable in the names of ${}^{\mathrm{v}}M_1$ and ${}^{\mathrm{v}}M_2$.

RESULTS AND DISCUSSION

We used data for C_3–C_8 alkanes from our previous paper.[9] The structure-boiling point modeling was based on the CROMRsel procedure.[37–40] This is a multivariate procedure, which selects the best possible model among the set of models obtained for a given number of parameters, the criterion being the standard error of estimate. The quality of models is expressed by fitted statistical parameters: the correlation coefficient r_{fit}, the standard error of estimate s_{fit} while F is the result of Fisher's test. The models were also cross-validated by using the leave-one-out procedure. Statistical parameters for the cross-validated models are denoted by r_{cv} and s_{cv}, where cv stands for the cross-validation procedure.

The standard errors of estimate, s_{fit} and s_{cv}, were computed using the following expressions:

$$s_{\mathrm{fit}} = \sqrt{[\sum_{i=1}^{N} (\mathrm{P}_i - \mathrm{P(fit)}_i^{\mathrm{est}})^2] / (N - I - 1)} \qquad (10)$$

$$s_{\mathrm{cv}} = \sqrt{[\sum_{i=1}^{N} (\mathrm{P}_i - \mathrm{P(cv)}_i^{\mathrm{est}})^2] / (N - I - 1)} \qquad (11)$$

where P_i denotes the values of a given experimental property, $\mathrm{P(fit)}_i^{\mathrm{est}}$ estimated values based on the fit statistical procedure, $\mathrm{P(cv)}_i^{\mathrm{est}}$ estimated values based on the leave-one-out cross-validation procedure, N is the number of data points used in the model building and I is the number of descriptors contained in the model.

The following results were obtained:

1. ${}^{\mathrm{v}}M_1^{[\lambda]}$

Note that ${}^{\mathrm{v}}M_1^{[\lambda]}$ is a variable Zagreb M_1 index with the optimum exponent λ.

(i) The best single-descriptor model

$$\mathrm{bp} = -108.9\ (\pm 4.5) + 21.84\ (\pm 0.50)\ {}^{\mathrm{v}}M_1^{[\lambda\ =\ 1/4]} \qquad (12)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.991 \quad r_{\mathrm{cv}} = 0.989$$
$$s_{\mathrm{fit}} = 5.75 \quad s_{\mathrm{cv}} = 6.15 \quad F = 1880$$

(ii) The best two-descriptor model:

– With p_3

$$\mathrm{bp} = -103.8\ (\pm 5.9) + 1.00\ (\pm 0.74)\ p_3 + 20.68\ (\pm 0.99)\ {}^{\mathrm{v}}M_1^{[\lambda\ =\ 1/4]} \qquad (13)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.991 \quad r_{\mathrm{cv}} = 0.989$$
$$s_{\mathrm{fit}} = 5.68 \quad s_{\mathrm{cv}} = 6.31 \quad F = 962$$

– With *twc*

$$\mathrm{bp} = -118.1\ (\pm 5.3) - 0.0071\ (\pm 0.0025)\ twc + 23.42\ (\pm 0.73)\ {}^{\mathrm{v}}M_1^{[\lambda\ =\ 1/4]} \qquad (14)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.992 \quad r_{\mathrm{cv}} = 0.991$$
$$s_{\mathrm{fit}} = 5.26 \quad s_{\mathrm{cv}} = 5.77 \quad F = 1125$$

(iii) The best three-descriptor model

$$\mathrm{bp} = -110.3\ (\pm 4.1) + 3.64\ (\pm 0.64)\ p_3 - 0.0154\ (\pm 0.0023)\ twc + 21.11(\pm 0.67)\ {}^{\mathrm{v}}M_1^{[\lambda\ =\ 1/4]} \qquad (15)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.996 \quad r_{\mathrm{cv}} = 0.995$$
$$s_{\mathrm{fit}} = 3.82 \quad s_{\mathrm{cv}} = 4.32 \quad F = 1432$$

It is interesting to note that, in all cases, the best model was always obtained with ${}^{\mathrm{v}}M_1^{[\lambda\ =\ 1/4]}$.

2. ${}^{\mathrm{v}}M_2^{[\lambda]}$

Note that ${}^{\mathrm{v}}M_2^{[\lambda]}$ is a variable Zagreb M_2 index with the optimum exponent λ.

(i) The best single-descriptor model

$$\mathrm{bp} = -112.3\ (\pm 3.6) + 50.49\ (\pm 0.90)\ {}^{\mathrm{v}}M_2^{[\lambda\ =\ -1/3]} \qquad (16)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.994 \quad r_{\mathrm{cv}} = 0.993$$
$$s_{\mathrm{fit}} = 4.48 \quad s_{\mathrm{cv}} = 4.87 \quad F = 3122$$

(ii) The best two-descriptor model:

– With p_3

$$\mathrm{bp} = -103.8\ (\pm 4.0) + 1.68\ (\pm 0.49)\ p_3 + 46.1\ (\pm 1.5)\ {}^{\mathrm{v}}M_2^{[\lambda\ =\ -1/3]} \qquad (17)$$

$$N = 38 \quad r_{\mathrm{fit}} = 0.996 \quad r_{\mathrm{cv}} = 0.995$$
$$s_{\mathrm{fit}} = 3.92 \quad s_{\mathrm{cv}} = 4.47 \quad F = 2046$$

– With *twc*

$$\mathrm{bp} = -112.4\ (\pm 4.4) - 0.0001\ (\pm 0.0020)\ twc + 50.5\ (\pm 1.3)\ {}^{v}M_2^{[\lambda = -1/3]} \quad (18)$$

$$N = 38 \quad r_{fit} = 0.994 \quad r_{cv} = 0.992$$
$$s_{fit} = 4.54 \quad s_{cv} = 5.26 \quad F = 1518$$

Because of the negligible contribution from the *twc*, this model is practically identical to a single-parameter model (16).

(iii) The best three-descriptor model

$$\mathrm{bp} = -105.9\ (\pm 3.4) + 3.19\ (\pm 0.56)\ p_3 - 0.0079\ (\pm 0.0020)\ twc + 46.1\ (\pm 1.2)\ {}^{v}M_2^{[\lambda = -1/3]} \quad (19)$$

$$N = 38 \quad r_{fit} = 0.997 \quad r_{cv} = 0.996$$
$$s_{fit} = 3.29 \quad s_{cv} = 4.03 \quad F = 1942.8$$

Similarly as in the case of the variable Zagreb M_1 index, the best models always contain ${}^{v}M_2$ with the exponent $\lambda = -1/3$.

The above results show that the variable Zagreb M_2 index produces slightly better models than the variable Zagreb M_1 index.

Table I gives a selection of the structure-boiling point models from the literature with up to three descriptors for C_3–C_8 alkanes.

Apparently, the variable Zagreb indices, with the optimal λ value, produce better single-descriptor structure-boiling point models than the original Zagreb indices, their modified forms and the overall Zagreb indices, and many other indices. They are comparable to a single descriptor model[8] based on the connectivity index (s_{fit} = 5.75 °C).[49] The two-descriptor model based on the variable Zagreb M_2 index with $\lambda = -1/3$ (s_{fit} = 3.92 °C) is better than most two-descriptor models in the literature, it is comparable to the model based on ${}^{1}\chi$ and M_2 indices[9] (s_{fit} = 3.84 °C) and is poorer than the Rücker-Rücker model[34] based on $\chi^{1/3}$ and mwc_5 (s_{fit} = 2.21 °C). The three-descriptor model with ${}^{v}M_2^{[\lambda = -1/3]}$ (s_{fit} = 3.29 °C) is comparable to some models based on three descriptors, but is somewhat poorer than the model[9] based on ${}^{1}\chi$, OM_1 and *twc* (s_{fit} = 2.57 °C) and much poorer than the model[34] based on p_3, $W^{0.25}$ and V (s_{fit} = 1.38 °C). Models with four and five different descriptors produce the standard error of estimate even lower than 1 °C.

TABLE I. Fitted statistical parameters of some structure-boiling point models with up to three descriptors for C_3–C_8 alkanes taken from the literature

Descriptor	I[a]	r_{fit}	s_{fit}	Ref.
${}^{0}M_1$[b]	1	0.875	20.3	8
${}^{0}M_2$[b]	1	0.985	7.2	8
TC[c]	1	0.753	27.6	41
TC1[c]	1	0.732	28.6	41
S[d]	1	0.795	25.4	41
${}^{0}\chi$[e]	1	0.954	12.5	41
${}^{1}\chi$[f]	1	0.990	5.75	9
^{0}TC,[g] ^{1}TC	2	0.9933	4.92	41
${}^{0}M_1$, ${}^{1}M_1$	2	0.989	6.22	8
${}^{0}M_2$, ${}^{1}M_2$	2	0.990	6.12	8
${}^{0}\chi$, ${}^{2}\chi$	2	0.9927	5.13	41
$\chi^{0.33}$,[h] mwc_5[i]	2		2.21	34
${}^{1}\chi$, M_2	2	0.996	3.84	9
^{0}TC, ^{1}TC, ^{1}TC1[j]	3	0.9962	3.75	41
${}^{0}\chi$, ${}^{2}\chi$, ${}^{5}\chi$	3	0.9943	4.58	41
${}^{1}\chi$, OM_1, *twc*	3	0.998	2.57	9
p_3,[k] $W^{0.25}$,[l] V[m]	3		1.38	34

[a] I = the number of descriptors in the model.
[b] ${}^{0}M_1$, ${}^{0}M_2$ = the overall Zagreb indices.[8]
[c] TC, TC1 = total values of topological complexity indices.[41]
[d] S = total number of connected subgraphs of a graph.[41]
[e] ${}^{0}\chi$ = the zero-order connectivity index.[42,43]
[f] ${}^{1}\chi$ = the first-order connectivity index.[44]
[g] ${}^{e}\chi$ (e = 0,1,...,E) = the connectivity indices from the zero-order to the E-order.[42,43] E is the total number of edges in a molecular graph.
[h] $\chi^{0.33}$ = cubic root of the connectivity index.[45]
[i] mwc_5 = molecular walk count of order 5.[34,46–48]
[j] ^{e}TC (e = 0,1,..,E), ^{e}TC1 (e = 1,2,...,E) = e^{th} order topological complexity indices.[41]
[k] p_3 = number of paths of length 3.[5,36]
[l] W^{α} = the fourth root of the Wiener index.[3,49]
[m] V = the number of vertices in a molecular graph.

CONCLUDING REMARKS

We note that the variable vertex-connectivity index[50] is formally identical to the variable Zagreb M_2 index. Thus, one may say that the meeting point of these two topological indices is reached in their variable forms: ${}^{v}M_2 = {}^{v}({}^{1}\chi)$. The reader should be reminded that the road to the first-order connectivity index (${}^{1}\chi$) was[9] the Zagreb M_2 index $\Rightarrow$ modified Zagreb M_2 index $\Rightarrow$ ${}^{1}\chi$. However, this road was not taken; the first order vertex-connectivity index was derived in quite a different way[44] than the Zagreb M_2 index.[1]

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SAŽETAK

O varijabilnim Zagrebačkim indeksima

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Predložena je nova inačica Zagrebačkih indeksa, uvedenih 1972., koja je nazvana varijabilni Zagrebački indeksi. Njihova uloga u modeliranju točke vrelišta nižih (C_3–C_8) alkana uspoređena je s izvornim Zagrebačkim indeksima i njihovim modifikacijama. Varijabilni Zagrebački indeksi vode do boljih jedno-deskriptorskih modela nego druge vrste Zagrebačkih indeksa, a sudjeluju u gradnji dobrih dvo- i tro-deskriptorskih modela.