Valence Connectivity versus Randić, Zagreb and Modified Zagreb Index: A Linear Algorithm to Check Discriminative Properties of Indices in Acyclic Molecular Graphs

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Valence connectivity in molecular graphs is described by 10-tuples \( \mu_{ij} \) where \( \mu_{ij} \) denotes the number of edges connecting vertices of valences \( i \) and \( j \). A shorter description is provided by 4-tuples containing the number of vertices and values of Randić, Zagreb and modified Zagreb indices. Surprisingly, these two descriptions are in one-to-one correspondence for all acyclic molecules of practical interest, i.e., for all those having no more than 100 atoms. This result was achieved by developing an efficient algorithm that is linear in the number of 10-tuples.

Key words: valence connectivity, acyclic molecular graphs, topological indices

INTRODUCTION

One of the central notions in chemistry is that of the valence of atoms. Atoms of various valences form chemical bonds. Let \( n_i \) denote the number of vertices of degree \( i \) and let \( \mu_{ij} \) denote the number of bonds whose terminal atoms are of valences \( i \) and \( j \). The collection of all \( \mu_{ij} \) is termed valence connectivity.\(^1\)\(^-\)\(^4\)

Molecules are conveniently represented by molecular graphs where hydrogen atoms are usually omitted.\(^5\)\(^-\)\(^6\) In most molecules, like those of organic chemistry valences are at most 4, and accordingly the valence connectivities are conveniently represented by 10-tuples of the form \( \mu = (\mu_{11}, \mu_{12}, \mu_{13}, \mu_{14}, \mu_{22}, \mu_{23}, \mu_{24}, \mu_{33}, \mu_{34}, \mu_{44}) \). Of course, \( \mu_{11} \neq 0 \) is only rarely encountered, like e.g. in a graph depicting ethylene. Graph theoretical terms are parallel to the chemical ones, and instead of molecules, atoms, bonds, valences, etc., one speaks respectively of graphs, vertices, edges, vertex degrees, etc.

When the topology of bonding in molecules is contracted to a number, one speaks of a molecular descriptor or topological index.\(^7\) Thus far, hundreds of topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.\(^8\)\(^-\)\(^9\)

Here, we consider three indices, which are fully defined by knowing only the valence connectivity in a graph \( G \). These are the Randić index, \( \chi \)\(^10\):

\[
\chi = \chi(G) = \sum_{i,j=1}^{n} \frac{\mu_{ij}(G)}{\sqrt{i \cdot j}},
\]

the Zagreb index, \( M_2 \)\(^11\):

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Besides, 10-tuples of \( n, \chi, M_2, \mu_6 \) represent another way of describing the topology of molecular graphs. Obviously, the knowledge of 10-tuples uniquely determines 4-tuples, but the opposite does not hold. From here on, we restrict ourselves to acyclic molecules, i.e., to trees, where \( l = n - 1 \) holds.

The main objective of this paper is to determine when 4-tuples uniquely determine 10-tuples in such graphs. In order to do so, an algorithm is developed here, which for fixed \( n \) checks whether there is one-to-one correspondence between 4- and 10-tuples. Trivial checking would require testing of all possible pairs of 10-tuples, i.e., it is quadratic in the number of 10-tuples. The algorithm presented here (after all 10-tuples of \( m_i \)'s are generated) is linear in that the number and the execution of this algorithm take about three hours on a PC with Celeron 800 processor.

RESULTS

First, we start with a few auxiliary results. Using the theory of the finite extensions of the field of rational numbers or simple, but tedious elementary calculation, it can be shown that:

\[
M_2 = M_2(G) = \sum_{i < j \leq 4} i \cdot j \cdot \mu_i(G) \tag{2}
\]

and the modified Zagreb index \( \ast M_2 \):

\[
\ast M_2 = \ast M_2(G) = \sum_{i < j \leq 4} \frac{\mu_i(G)}{i \cdot j}.
\]

The number of vertices, \( n \), and the number of edges in \( G, l \), are simply related to \( \mu_i \)'s as follows:

\[
n = n(G) = \sum_{i < j \leq 4} \left( \frac{1 + \frac{1}{i}}{j} \right) \cdot \mu_i(G) \tag{4}
\]

\[
l = l(G) = \sum \mu_i(G) \tag{5}
\]

From the last Lemma, it directly follows that:

\[
\text{Lemma 2.} \quad \text{Let } G \text{ be any molecular graph. Then the numbers } a(G), b(G), c(G) \text{ and } d(G) \text{ are uniquely determined by } \chi(G).
\]

Let us prove:

\[
\text{Lemma 3.} \quad \text{Let } G_1 \text{ and } G_2 \text{ be two molecular graphs such that:}
\]

\[
\{ \left( \chi(G_1) = \chi(G_2) \right) \text{ and } (M_2(G_1) = M_2(G_2)) \text{and}
\]

\[
\{(\ast M_2(G_1) = \ast M_2(G_2)) \text{ and } (n_2(G_1) = n_2(G_2)) \}
\]

\[
\Rightarrow (\mu(G_1) = \mu(G_2)). \tag{6}
\]

then

1) \( \mu_{11}(G_1) = 0 \) and \( \mu_{11}(G_2) = 0 \)
2) \( n_2(G_1) \neq 0 \) and \( n_2(G_2) \neq 0 \)
3) \( n_3(G_1) \neq 0 \) and \( n_3(G_2) \neq 0 \).

\[
\text{Proof.} \quad \text{Note that for each molecular graph } G \text{ with at least three vertices, we have } \mu_{11}(G) = 0 \text{ and that single graph with 2 vertices is a path of length one, and hence indeed 1) holds.}
\]

Now, let us prove 2). Suppose, in contrast, that there are graphs \( G_1 \) and \( G_2 \) that satisfy (6), but do not satisfy relation 2). Denote \( a = a(G_1) = a(G_2), b = b(G_1) = b(G_2) \) and analogously for \( c, d, M_2, \ast M_2 \) and \( n \). Without loss of generality, we may assume that \( n_2(G_i) = 0 \). It follows that \( \mu_{12}(G_1) = \mu_{22}(G_1) = \mu_{23}(G_1) = \mu_{24}(G_1) \), hence \( b = d = 0 \), and therefore \( \mu_{12}(G_2) = \mu_{24}(G_2) = \mu_{23}(G_2) = 0 \). Note that for each \( i \in \{1, 2\} \), we have:

\[
6 \mu_{14}(G_i) + 6 \mu_{12}(G_i) + 4 \mu_{35}(G_i) + 3 \mu_{44}(G_i) = a
\]

\[
2 \mu_{13}(G_i) + \mu_{34}(G_i) = c
\]

\[
\frac{\mu_{13}(G_i) + \mu_{14}(G_i) + 2 \mu_{22}(G_i)}{2} + \frac{\mu_{13}(G_i) + 2 \mu_{35}(G_i) + \mu_{44}(G_i)}{3} + \frac{\mu_{14}(G_i) + \mu_{34}(G_i) + 2 \mu_{44}(G_i)}{4} = n
\]

\[
\mu_{11}(G_i) + \mu_{14}(G_i) + \mu_{22}(G_i) + \mu_{33}(G_i) + \mu_{34}(G_i) + \mu_{44}(G_i) = n - 1
\]
3\mu_{13}(G_i) + 4\mu_{14}(G_i) + 4\mu_{22}(G_i) + 9\mu_{33}(G_i) + 12\mu_{34}(G_i) + 16\mu_{44}(G_i) = M_2

\frac{1}{3}\mu_{13}(G_i) + \frac{1}{4}\mu_{14}(G_i) + \frac{1}{4}\mu_{22}(G_i) + \frac{1}{9}\mu_{33}(G_i) + \\
\frac{1}{12}\mu_{34}(G_i) + \frac{1}{16}\mu_{44}(G_i) = *M_2

i.e., a system of 6 equations in 6 unknowns \mu_{13}(G_i), \mu_{14}(G_i), \mu_{22}(G_i), \mu_{33}(G_i), \mu_{34}(G_i) and \mu_{44}(G_i). Note that the matrix of the system has a rank equal to 6; hence, there is a unique solution to these equations, and this is in contradiction with \mu(G_1) \neq \mu(G_2).

Let us prove 3). Suppose, in contrast, that there are graphs \( G_1 \) and \( G_2 \) such that:

1) \( m_1 = (1,0,0,0,0,0) \)

2) \( m_2 = (0,2,0,0,0,0,0) \)

3) \( (m_{11} = 0) \) and \( (n_{23}, n_{34} \in N_0) \) and \((q \geq 0)\) and \((m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1)\) and \([m_{12} + m_{23} + m_{24} \neq 0]\) or \[(m_{22} = 0)\] and one of the following holds:

3.1) \( m_{44} \leq n_4 - 1 \) and \((m_{33} \leq n_3 - 1)\) and \((q + m_{33} - m_{24} \leq n_3 - 1)\) and \((q + m_{44} - m_{23} \leq n_4 - 1)\)

3.2) \( n_3 = 0 \)

3.3) \( n_4 = 0 \)

where

\( n_2 = (m_{12} + 2m_{22} + m_{23} + m_{24})/2 \)
\( n_3 = (m_{13} + m_{23} + 2m_{33} + m_{34})/3 \)
\( n_4 = (m_{14} + m_{24} + m_{34} + 2m_{44})/4 \)
\( q = (m_{23} + m_{24} - m_{12})/2 \)

Now, it readily follows that:

Lemma 5. – Let \( m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in N_0^{10} \). There are acyclic molecular graphs \( G_1 \) and \( G_2 \), such that \( \mu(G_1) = m, \nu(G_1) = \nu(G_2), M_2(G_1) = M_2(G_2), *M_2(G_1) = *M_2(G_2), \chi(G_1) = \chi(G_2) \) and \( \mu(G_1) \neq \mu(G_2) \) only if \( (m_{11} = 0) \) and \((n_{23}, n_{34} \in N_0)\) and \((q \geq 0)\) and \((m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1)\) and \((m_{12} + m_{23} + m_{24} > 0)\) and \((m_{33} \leq n_3 - 1)\) and \((q + m_{33} - m_{24} \leq n_3 - 1)\) and one of the following holds:

1) \( m_{44} \leq n_4 - 1 \) and \((q + m_{44} - m_{23} \leq n_4 - 1)\)

2) \( n_4 = 0 \)

where

\( n_2 = (m_{12} + 2m_{22} + m_{23} + m_{24})/2 \)
\( n_3 = (m_{13} + m_{23} + 2m_{33} + m_{34})/3 \)
\( n_4 = (m_{14} + m_{24} + m_{34} + 2m_{44})/4 \)
\( q = (m_{23} + m_{24} - m_{12})/2 \)

Theorem 6. – Let \( A, B, C, D, n, M_2, *M_2 \in N_0 \). There are acyclic molecular graphs \( G_1 \) and \( G_2 \), such that:

\( a(G_1) = a(G_2) = A; b(G_1) = b(G_2) = B; \)
\( c(G_1) = c(G_2) = C; d(G_1) = d(G_2) = D; \)
\( \nu(G_1) = \nu(G_2) = n; M_2(G_1) = M_2(G_2) = M_2; *M_2(G_1) = *M_2(G_2) = *M_2, \mu(G_1) \neq \mu(G_2) \)

if and only if

In our paper,\(^2\) it is shown that:

Theorem 4. – Let \( m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in N_0^{10} \) where \( N_0^{10} \) is the set of 10-tuples of nonnegative integers. Then, there is an acyclic molecu-
and
\[ e \in Z, \]
where
\[ Q = 144 \cdot M_2 \]
\[ e = A - (6 + 6B + 6C + 6M_2 + 6n + Q) \]
\[ 12 \]
and \( \alpha(R) \) is 1 if relation \( R \) holds and 0 otherwise. \( \text{card} \) denotes the cardinality of the set and \( Z \) stands for the set of integers.

**Proof.** From the previous results, it follows that graphs \( G_1 \) and \( G_2 \) with the required properties exist if and only if there are:
\[ m_i = (m_{11,i}, m_{12,i}, m_{13,i}, m_{14,i}, m_{22,i}, m_{23,i}, m_{24,i}, m_{33,i}, m_{34,i}, m_{44,i}) \in \mathcal{K}^{10}_0, i = 1, 2 \]
such that:

i.1) \( m_{ui,v} \in Z \), for each \( 1 \leq u \leq v \leq 4 \)

i.2) \( m_{ui,v} \geq 0 \) for each \( 1 \leq u \leq v \leq 4, m_{11,i} = 0 \)

i.3) \( n_{2,i} \in Z \)

i.4) \( n_{3,i} \in Z \)

i.5) \( n_{4,i} \in Z \)

i.6) \( q_i \in Z \)

i.7) \( q_i \geq 0 \)

i.8) \( A = 6m_{14,i} + 6m_{22,i} + 4m_{33,i} + 3m_{44,i} \)

i.9) \( B = 2m_{12,i} + m_{14,i} \)

i.10) \( C = 2m_{13,i} + m_{34,i} \)

i.11) \( D = m_{23,i} \)

i.12) \( m_{33,i} + m_{34,i} + q = n_{3,i} + n_{4,i} - 1 \)

i.13) \( n_{1,i} + n_{2,i} + n_{3,i} + n_{4,i} = n \)

i.14) \( 2m_{12,i} + 3m_{13,i} + 4m_{14,i} + 4m_{22,i} + 6m_{33,i} + 8m_{44,i} + 9m_{33,i} + 12m_{34,i} + 16m_{44,i} = M_2 \)

i.15) \( \frac{1}{2} m_{12,i} + \frac{1}{3} m_{13,i} + \frac{1}{4} m_{14,i} + \frac{1}{4} m_{22,i} + \frac{1}{4} m_{23,i} + \frac{1}{6} m_{24,i} + \frac{1}{8} m_{33,i} + \frac{1}{9} m_{34,i} + \frac{1}{12} m_{44,i} = *M_2 \)

i.16) \( m_{12,i} + m_{23,i} + m_{24,i} > 0 \)

i.17) \( m_{33,i} \leq n_{3,i} - 1 \)

i.18) \( q_i + m_{33,i} - m_{24,i} \leq n_{1,i} - 1 \)

i.19) \( n_{4,i} = 0 \) or \( (m_{44,i} \leq n_{4,i} - 1 \) and \( q + m_{44,i} - m_{23,i} \leq n_{4,i} - 1) \)

(7) \( 20) m_1 \neq m_2 \)
where
\[ n_{1,i} = m_{1,2,i} + m_{1,3,i} + m_{1,4,i} \]
\[ n_{2,i} = (m_{1,2,i} + 2m_{2,2,i} + m_{2,3,i} + m_{2,4,i}) / 2 \]
\[ n_{3,i} = (m_{1,3,i} + m_{2,3,i} + 2m_{3,3,i} + m_{3,4,i}) / 3 \]
\[ n_{4,i} = (m_{1,4,i} + m_{2,4,i} + m_{3,4,i} + 2m_{4,4,i}) / 4 \]
\[ q_i = (m_{2,3,i} + m_{2,4,i} + m_{2,4,i}) / 2 . \]

Note that relations i,3) and i,8) – i,15) are equivalent to:

i,1*) \( m_{1,1,i} = 0 \)
i,2*) \( m_{1,2,i} = (-24 - 10A - 42B - 36C - 48D + 24n + Q) / 12 - m_{4,4,i} / 4 \)
i,3*) \( m_{1,3,i} = (-348 - 80A - 342B - 264C - 396D - 12M_2 + 348n + 5Q) / 24 + 13m_{4,4,i} / 8 \)
i,4*) \( m_{1,4,i} = (348 + 56A + 234B + 180C + 276D + 12M_2 - 204n - 5Q) / 36 - 15m_{4,4,i} / 12 \)
i,5*) \( m_{2,2,i} = (456 + 131A + 558B + 450C + 636D + 12M_2 - 528n - 8Q) / 18 - 7m_{4,4,i} / 6 \)
i,6*) \( m_{2,3,i} = D \)
i,7*) \( m_{2,4,i} = (24 + 10A + 48B + 36C + 48D - 24n - Q) / 6 + m_{4,4,i} / 2 \)
i,8*) \( m_{3,3,i} = (-420 - 104A - 450B - 360C - 516D - 12M_2 + 420n + 7Q) / 8 + 21m_{4,4,i} / 8 \)
i,9*) \( m_{3,4,i} = (348 + 80A + 342B + 276C + 396D + 12M_2 - 348n - 5Q) / 15m_{4,4,i} / 4 \)

Note that \( m_{1,3,i} \in N \), hence:
\[ -348 - 80A - 342B - 264C - 396D - 12M_2 + 348n + 5Q = 0 \] (mod 3)
or equivalently,
\[ A \equiv Q \pmod{3} . \]

Note also that \( 33n_3 + 87n_4 \in Z \), hence:
\[ -270 - 137A - 582B - 474C - 672D + 6M_2 + 618n + 5Q = 0 \] (mod 4)
or equivalently:
\[ A \equiv 2 + 2B + 2C + 2M_2 + 2n + Q \pmod{4} . \]

We can rewrite (8)–(9) as:
\[ 4A = 4Q \pmod{12} \]
\[ 3A \equiv 6 + 6B + 6C + 6M_2 + 6n + 3Q \pmod{12} \]

It follows that:
\[ A \equiv 6 + 6B + 6C + 6M_2 + 6n + Q \pmod{12} \]

therefore \( e \in Z \). Substituting this in relations i,1*) – i,8*), we get:
\[ n_{3,i} = \frac{1}{24} \left( 1740 + 1906B + 1744C + 908D + 2216e + 1124M_2 + 380n + 173Q - 25m_{4,4,i} \right) . \]

This implies that:
\[ m_{4,4,i} = 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q \pmod{24} . \]

Hence, there are numbers such that:
\[ m_{4,4,i} = 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q + 24x_i \]

It readily follows that relations i,1*) – i,8*) can be replaced by:
i,1*) \( m_{1,1,i} = 0 \)
i,2*) \( m_{1,2,i} = -10 - 11B - 12C - 9D - 12e - 10M_2 - 8n - 2Q - 6x_i \)
i,3*) \( m_{1,3,i} = -15 - 18B - 5C + 16D - 27e + 12M_2 + 27n + 5Q + 39x_i \)
i,4*) \( m_{1,4,i} = 5B - 3C - 2(-3 + 7D - 5e + 6M_2 + 9n + 2Q + 13x_i) \)
i,5*) \( m_{2,2,i} = 55 + 63B + 50C + 12D + 78e + 21M_2 - 9n + Q - 28x_i \)
i,6*) \( m_{2,3,i} = D \)
i,7*) \( m_{2,4,i} = 23B + 2(10 + 12C + 9D + 12e + 10M_2 + 8n + 2Q + 6x_i) \)
i,8*) \( m_{3,3,i} = -99 - 108B - 81C + 12D - 135e - 27M_2 + 27n + Q + 63x_i \)
i,9*) \( m_{3,4,i} = 36B + 11C - 2(-15 + 16D - 27e + 12M_2 + 27n + 5Q + 39x_i) \)
i,10*) \( m_{4,4,i} = 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q + 24x_i \)
i,11*) \( x_i \in Z \)

where
\[ x_i = \frac{1}{24} \left( m_{4,4,i} - (12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q) \right) . \]

It is obvious that relation i,1) is satisfied and since the following holds:
\[ n_{2,i} = 60 + 69B + 56C + 17D + 84e + 26M_2 - 5n + 2Q - 25x_i \]
\[ n_{3,i} = -61 - 66B - 52C - 13D - 81e - 22M_2 + 9n - Q + 29x_i \]
\[ n_{4,i} = 20 + 21B + 16C + 3D + 26e + 6M_2 - 4n - 11x_i \]
\[ q_i = 30 + 34B + 36C + 28D + 36e + 30M_2 + 24n + 6Q + 18x_i \]
relations i,3) – i,6) are satisfied, too. Relations i,2), i,7) and i,16) – i,18) are equivalent to i,12):

\[
\begin{align*}
&5/13 + 6B/13 + 5C/39 - 16D/39 + 9e/13 - 4M_z/13 - 9n/13 - 7Q/156, \\
&-5/3 - 23B/21 - 12 - 2C - 3D/12 - 2e - 2e - 2e - 5M_z/3 - 4n + 3 - 5Q/6, \\
&11/7 + 12B/7 + 9C/7 + 4D/21 + 15e/7 + 3M_z/7 + 3n/7 + 13Q/252, \\
&-1/2 - 5B/12 - 2C - 3 - 5D/6 - e - 3 - 5M_z + 6 - 5n + 6 - 7Q/24, \\
&-5/3 - 17B + 9 - 2C - 14D/9 - 2e - 5M_z/3 - 3 - 4n/3 - 3 - 5Q/6, \\
&-5/3 - 1B/6 - 2C - 3D/2 - 2e - 5M_z/3 - 4n + 3 - 5Q/6, \\
&3/13 + 5B/26 + 3C/26 - 7D/13 + 5e/13 - 6M_z/13 - 9n - 13 - 3Q/52, \\
&55/28 + 9B/4 + 25C/14 + 3D/7 + 39e/14 + 3M_z/4 - 9n + 28 + 4Q/56, \\
&5/13 + 6B/13 + 11C/78 - 16D/39 + 9e/13 - 4M_z/13 - 9n + 13 - 17Q/156, \\
&37/34 + 2B/17 + 29C/34 - 3D/34 + 27e/17 + 5M_z/34 - 9n + 17 + 127Q/136, \\
&27/40 + 3B/40 + 17C/40 - 11D/40 + 21e/20 - 5 - 13n + 20 + 143Q/160,
\end{align*}
\]

Note that statements (connected by or) in i,19) are mutually exclusive, i.e., i,19) is equivalent to:

i,13(a) exactly one of the following statements is true:

\[
\begin{align*}
i,13^{\text{a)}a}) x &= (20 + 21B + 16C + 3D + 26e + 6M_z - 4n) / 11, \\
i,13^{\text{a)}}b) x &\leq \text{ min} \ [1/5 + 1B/35 - 17D/35 + 18e/35 - 2M_z/5 - 24n/35 - Q/5, \\
\end{align*}
\]

Note that all numbers \(m_{11}, \ldots, m_{44}\) are uniquely determined by the value of \(x_i\), and hence relation 20) is equivalent to:

i,14) \(x_i \neq x_j\)

We can conclude that there are graphs \(G_1\) and \(G_2\) with the required properties if and only if there are integers \(x_1\) and \(x_2\), such that i,12) (i,14) hold. The existence of these numbers is equivalent to:

\[\text{card}(S) \geq 2\]

where

\[S = \begin{pmatrix} 5/13 + 6B/13 + 5C/39 - 16D/39 + 9e/13 - 4M_z/13 - 9n/13 + 7Q/156, \\
-5/3 - 23B/21 - 12 - 2C - 3D/12 - 2e - 2e - 2e - 5M_z/3 - 4n + 3 - 5Q/6, \\
11/7 + 12B/7 + 9C/7 + 4D/21 + 15e/7 + 3M_z/7 + 3n/7 + 13Q/252, \\
-1/2 - 5B/12 - 2C - 3 - 5D/6 - e - 3 - 5M_z + 6 - 5n + 6 - 7Q/24, \\
-5/3 - 17B + 9 - 2C - 14D/9 - 2e - 5M_z/3 - 3 - 4n/3 - 3 - 5Q/6, \\
-5/3 - 1B/6 - 2C - 3D/2 - 2e - 5M_z/3 - 4n + 3 - 5Q/6, \\
3/13 + 5B/26 + 3C/26 - 7D/13 + 5e/13 - 6M_z/13 - 9n - 13 - 3Q/52, \\
55/28 + 9B/4 + 25C/14 + 3D/7 + 39e/14 + 3M_z/4 - 9n + 28 + 4Q/56, \\
5/13 + 6B/13 + 11C/78 - 16D/39 + 9e/13 - 4M_z/13 - 9n + 13 - 17Q/156, \\
37/34 + 2B/17 + 29C/34 - 3D/34 + 27e/17 + 5M_z/34 - 9n + 17 + 127Q/136, \\
27/40 + 3B/40 + 17C/40 - 11D/40 + 21e/20 - 5 - 13n + 20 + 143Q/160,
\end{pmatrix}\]

\[\text{Now we utilize Theorem 6 to check whether the following holds for acyclic graphs:}
\]

\[\begin{align*}
&\left((\varphi(G_1) = \varphi(G_2)) \text{ and } (M_2(G_1) = M_2(G_2)) \text{ and } (n = n(G_1) = n(G_2))\right) \\
&\Rightarrow (\mu(G_1) = \mu(G_2))
\end{align*}\]

\[\text{i.e., for which values of } n \text{ 4-tuples uniquely determine 10-tuples. An algorithm is given in Ref. 2 that for given } n \text{ generates the set } \Gamma_n \text{ of all 10-tuples } m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}), \text{ which are 10-tuples (i.e., } \mu(G) = m) \text{ of acyclic graphs with } n \text{ vertices. We use this algorithm in the first line of the pseudocode of the algorithm developed here.}
\]

\[\text{Let us denote the left hand side of inequality (7) by } T(A, B, C, D, n, M_2, *M_2). \text{ Now, we demonstrate our algorithm:}
\]

\[\begin{align*}
&\text{ALGORITHM}
\end{align*}\]
1) Input $n$
2) For each $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33},$
$m_{34}, m_{44}) \in \Gamma_n$
2.1) $A = m_{11} + 6m_{14} + 6m_{22} + 4m_{33} + 3m_{44}$
2.2) $B = 2m_{12} + m_{24}$
2.3) $C = 2m_{13} + m_{34}$
2.4) $D = m_{23}$
2.5) $M_2 = m_{11} + 2m_{12} + 3m_{13} + 4m_{14} + 4m_{22} + 6m_{23} + 8m_{24} + 9m_{33} + 12m_{34} + 16m_{44}$
2.6) *$M_2 = m_{11} + \frac{1}{2} m_{12} + \frac{1}{3} m_{13} + \frac{1}{4} m_{14} + \frac{1}{4} m_{22} +$
$\frac{1}{6} m_{23} + \frac{1}{8} m_{24} + \frac{1}{9} m_{33} + \frac{1}{12} m_{34} + \frac{1}{16} m_{44}$
2.7) Calculate $T(A, B, C, D, n, M_2, *M_2)$
2.8) If $T(A, B, C, D, n, M_2, *M_2) < 1$ then Error
2.9) If $T(A, B, C, D, n, M_2, *M_2) \geq 2$
2.9.1) Output: There are graphs $G_1$ and $G_2$ with $n$ vertices such that
\[
\begin{align*}
(\mu(G_1)) &\neq (\mu(G_2)) \\
(\mu(G_1)) = &\mu(G_2))
\end{align*}
\]
2.9.2) Output $A, B, C, D, M_2,$ *$M_2$ and exit
3) Output:
\[
\begin{align*}
(\mu(G_1)) = &\mu(G_2))
\end{align*}
\]
Note that line 2.8) does not solve the required problem, but it is a useful control, which verifies that the algorithm works correctly.

APPLICATIONS

The number of 10-tuples grows rapidly with $n$. Therefore, we have tested $n$ from 3 up to 100 and have found that for all these values 4-tuples uniquely determine 10-tuples of acyclic graphs. The procedure could be continued for higher values of $n$, but for some of these values 4-tuples cannot determine uniquely 10-tuples. That it is so shows the following example of two graphs $G_1$ and $G_2$ with $n = n(G_1) = n(G_2) = 241$:
\[
\begin{align*}
\alpha(G_1) &= \alpha(G_2) = 684; \\
\beta(G_1) &= \beta(G_2) = 12; \\
\gamma(G_1) &= \gamma(G_2) = 150; \\
\delta(G_1) &= \delta(G_2) = 6; \\
*M_2(G_1) &= *M_2(G_2) = 7344/144; \\
M_2(G_1) &= M_2(G_2) = 1548; \\
\mu(G_1) &= (0, 6, 36, 78, 36, 6, 0, 78, 0) \neq \\
\mu(G_2) &= (0, 0, 75, 52, 8, 6, 12, 63, 0, 24).
\end{align*}
\]

We represent these two graphs by the following figures:

There may be some lower values of $n$ where such a situation is encountered, but we leave it as an open problem.

CONCLUSIONS

Here, we consider two kinds of objects able to model valence connectivities: 10-tuples and 4-tuples containing the Randić, Zagreb, modified Zagreb indices and the number of vertices. A question is raised here whether there is one-to-one correspondence among 4- and 10-tuples for acyclic molecular graphs with a fixed number of vertices, and an algorithm is developed here which is able to answer this question. The algorithm is linear in the number of 10-tuples. The exhaustive computations have shown that the above one-to-one correspondence holds at least for all acyclic graphs with up to 100 vertices.

REFERENCES

3. D. Veljan and D. Vukičević, unpublished work.
SAŽETAK

Odnos susjednosti valencija i Randićevog, Zagrebačkoga i modificiranoga Zagrebačkoga indeksa: Linearni algoritam za provjeru diskriminativnih svojstava indeksa u acikličkim grafovima

Damir Vukičević i Ante Graovac

Susjednost valencija u molekularnim grafovima opisana je desetorkama $\mu_{ij}$ gdje $\mu_{ij}$ označava broj bridova koji povezuju čvorove valencija $i$ i $j$. Kraći opis susjednosti daju četvorke čiji su elementi broj vrhova u grafu i vrijednosti Randićevoga, Zagrebačkoga i modificiranoga Zagrebačkoga indeksa. Iznenadjuje da su ova dva opisa u obostrano jednoznačnoj korespondenciji za sve acikličke molekule od praktičnog interesa, tj. za sve one koje sadrže najviše do 100 atoma. Ovaj rezultat je dobiven primjenom ovdje razvijenog i opisanog algoritma koji je linearan u broju desetorki $\mu_{ij}$.