Calculating degree-based topological indices of dominating David derived networks

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Abstract: An important area of applied mathematics is the Chemical reaction network theory. The behavior of real world problems can be modeled by using this theory. Due to applications in theoretical chemistry and biochemistry, it has attracted researchers since its foundation. It also attracts pure mathematicians because it involves interesting mathematical structures. In this report, we compute newly defined topological indices, namely, Arithmetic-Geometric index (AG₁ index), SK index, SK₁ index, and SK₂ index of the dominating David derived networks [1–5].

Keywords: Network, Randić index, degree-based topological index

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1 Introduction

Chemical graph theory is a branch of graph theory in which a chemical compound is represented by simple graph called molecular graph in which vertices are atoms of compound and edges are the atomic bounds. A graph is connected if there is at least one connection between its vertices. If a graph does not contain any loop or multiple edge then it is called a network. Between two vertices u and v, the distance is the shortest path between them and is denoted by \( d(u, v) = d_G(u, v) \) in graph G. For a vertex v of G the “degree” \( d_v \) is the number of vertices attached with it. The degree and valence in chemistry are closely related with each other. We refer the book [6] for more details. Now a day another emerging field is Cheminformatics, which helps to predict biological activities with the relationship of Structure-property and quantitative structure-activity. Topological indices and Physico-chemical properties are used in prediction of bioactivity if underlined compounds are used in these studies [7–11].

A number that describe the topology of a graph is called topological index. In 1947, the first and most studied topological index was introduced by Weiner [12]. For more details about this index can be found in [13, 14]. In 1975, Milan Randić introduced the Randić index [15]. Bollobas et al. [16] and Amic et al. [17] in 1998, working independently defined the generalized Randić index. This index was studied by both mathematicians and chemists [18–28]. The first and the second Zagreb indices are defined as

\[
M_1(G) = \sum_{uv \in E(G)} (d_u + d_v),
\]

and

\[
M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).
\]

(see [30–34]). Sum connectivity index is defined as

\[
\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}},
\]

and modified Randić index is defined as

\[
R'(G) = \sum_{uv \in E(G)} \frac{1}{\max \{d_u, d_v\}}.
\]

Shigehalli and Kanabur [35] introduced following new degree-based topological indices: Arithmetic-Geometric (AG₁) index

\[
AG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2 \sqrt{d_u d_v}},
\]
SK(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2},
SK_1(G) = \sum_{uv \in E(G)} \frac{d_u \times d_v}{2},
SK_2(G) = \sum_{uv \in E(G)} \left( \frac{d_u + d_v}{2} \right)^2.

For more literature review, see Ref. [36–38].
In this report, we aim to compute degree-based topological indices of dominating David derived networks of first type, second type and third type. These networks are constructed and studied in [1–5].

2 Main results

In this section we present our computational results.

**Theorem 2.1.** Let \(D_1(n)\) be the Dominating David Derived Network of 1st type. Then

1. \(\chi(D_1(n)) = \frac{10008}{1000} \cdot n^2 - \frac{2963}{100} \cdot n + \frac{986}{100},\)
2. \(R'(D_1(n)) = 21n^2 - 21n + \frac{22}{3},\)
3. \(AG_1(D_1(n)) = (45 + 21\sqrt{3})n^2 - \frac{8179}{100} \cdot n + \frac{2819}{100},\)
4. \(SK(D_1(n)) = 297n^2 - 341n + 121,\)
5. \(SK_1(D_1(n)) = \frac{1089}{2} \cdot n^2 - \frac{1357}{2} \cdot n + \frac{501}{2},\)
6. \(SK_2(D_1(n)) = 1098n^2 - 1342n + 490.\)

**Proof.** In dominating derived network \(D_1(n)\) (see Figure 1) there are six type of edges in \(E(D_1(n))\) based on the degree of end vertices, i.e.

- \(E_1(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 2, \ d_v = 2\},\)
- \(E_2(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 2, \ d_v = 3\},\)
- \(E_3(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 2, \ d_v = 4\},\)
- \(E_4(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 3, \ d_v = 2\},\)
- \(E_5(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 3, \ d_v = 3\},\)
- \(E_6(D_1(n)) = \{uv \in E(D_1(n)) : d_u = 4, \ d_v = 4\}.

It can be observed from Figure 1, that

\[
\begin{align*}
|E_1(D_1(n))| &= 4n, \\
|E_2(D_1(n))| &= 4n - 4, \\
|E_3(D_1(n))| &= 28n - 16, \\
|E_4(D_1(n))| &= 9n^2 - 13n + 5, \\
|E_5(D_1(n))| &= 36n^2 - 56n + 24, \\
|E_6(D_1(n))| &= 36n^2 - 52n + 20.
\end{align*}
\]

Now,

\[
\begin{align*}
\chi(D_1(n)) &= \sum_{uv \in E(D_1(n))} \frac{1}{\sqrt{d_u + d_v}}, \\
R'(D_1(n)) &= \sum_{uv \in E(D_1(n))} \frac{\max\{d_u, d_v\}}{\sqrt{d_u + d_v}}, \\
AG_1(D_1(n)) &= \sum_{uv \in E(D_1(n))} \frac{d_u + d_v}{\sqrt{d_u + d_v}}, \\
SK(D_1(n)) &= \sum_{uv \in E(D_1(n))} \frac{d_u + d_v}{2}.
\end{align*}
\]

Note:

\[
\begin{align*}
|E_1(D_1(n))| &= 4n, \\
|E_2(D_1(n))| &= 4n - 4, \\
|E_3(D_1(n))| &= 28n - 16, \\
|E_4(D_1(n))| &= 9n^2 - 13n + 5, \\
|E_5(D_1(n))| &= 36n^2 - 56n + 24, \\
|E_6(D_1(n))| &= 36n^2 - 52n + 20.
\end{align*}
\]

Figure 1: Dominating David derived network of first type \(D_1(2)\)
It can be observed from Figure 2 that

\[ SK_1(D_1(n)) = \sum_{uv \in \bar{E}(D_1(n))} \frac{d_u d_v}{2} \]
\[ = |E_1(D_1(n))| \left( \frac{2 \cdot 2}{2^3} \right) + |E_2(D_1(n))| \left( \frac{2 \cdot 2}{2^3} \right) \]
\[ + |E_3(D_1(n))| \left( \frac{2 \cdot 2}{2^3} \right) + |E_4(D_1(n))| \left( \frac{2 \cdot 2}{2^3} \right) \]
\[ + |E_5(D_1(n))| \left( \frac{2 \cdot 2}{2^3} \right) \]
\[ = 4n \left( \frac{2}{2^3} \right) + (4n - 4) \left( \frac{2}{2^3} \right) + (28n - 16) \left( \frac{2}{2^3} \right) \]
\[ + (36n^2 - 52n + 20) \left( \frac{2}{2^3} \right) \]
\[ = \frac{1098n^2}{2} - 1342n + 490. \]

**Theorem 2.2.** Let \( D_2(n) \) be the dominating David derived network of 2nd type. Then
1. \( \chi(D_2(n)) = \frac{24318n^2 - 3595n + 1229}{100} \),
2. \( R'(D_2(n)) = 24n^2 - \frac{76n}{9} + 9, \)
3. \( AG_1(D_2(n)) = \frac{9074n^2 - 9733n + 3340}{100} \),
4. \( SK_2(D_2(n)) = 315n^2 - 367n + 131, \)
5. \( SK_1(D_2(n)) = 558n^2 - 698n + 258, \)
6. \( SK_2(D_2(n)) = \frac{2595n^2}{2} - \frac{2775n}{2} + 1015. \)

**Proof.** In dominated derived network \( D_2(n) \)(figure 2) there are five type of edges in \( E(D_2(n)) \) based on the degree of end vertices. i.e.

\[ E_1(D_2(n)) = \{ uv \in E(D_2(n)) : d_u = 2, d_v = 2 \}, \]
\[ E_2(D_2(n)) = \{ uv \in E(D_2(n)) : d_u = 2, d_v = 3 \}, \]
\[ E_3(D_2(n)) = \{ uv \in E(D_2(n)) : d_u = 2, d_v = 4 \}, \]
\[ E_4(D_2(n)) = \{ uv \in E(D_2(n)) : d_u = 3, d_v = 4 \}, \]
\[ E_5(D_2(n)) = \{ uv \in E(D_2(n)) : d_u = 4, d_v = 4 \}. \]

It can be observed from figure 2 that

\[ |E_1(D_2(n))| = 4n, \]
\[ |E_2(D_2(n))| = 18n^2 - 22n + 6, \]
\[ |E_3(D_2(n))| = 28n - 16, \]
\[ |E_4(D_2(n))| = 36n^2 - 56n + 24, \]
\[ |E_5(D_2(n))| = 36n^2 - 52n + 20. \]

Now,
Theorem 2.3. Let $D_3(n)$ be the dominating David derived network of 3rd type. Then

1. $\chi(D_3(n)) = (6\sqrt{3} + 18\sqrt{2}) n^2 - \frac{6434}{109} n + 11\sqrt{2}$,
2. $R'(D_3(n)) = 27n^2 - 30n + 11$,
3. $AG_1(D_3(n)) = (72 + 27\sqrt{2}) n^2 - \frac{1228}{109} n + 44$,
4. $SK(D_3(n)) = 396n^2 - 484n + 176$,
5. $SK_1(D_3(n)) = 720n^2 - 936n + 352$,
6. $SK_2(D_3(n)) = 1476n^2 - 1892n + 704$.

Proof. In dominating derived network $D_3(n)$ (Figure 3) there are three type of edges in $E(D_3(n))$ based on the degree of end vertices. i.e.

- $E_1(D_3(n)) = \{uv \in E(D_3(n)) : d_u = 2, d_v = 2\}$,
- $E_2(D_3(n)) = \{uv \in E(D_3(n)) : d_u = 2, d_v = 4\}$,
- $E_3(D_3(n)) = \{uv \in E(D_3(n)) : d_u = 4, d_v = 4\}$.

It can be observed from figure 3 that

- $|E_1(D_3(n))| = 4n$,
- $|E_2(D_3(n))| = 36n^2 - 20n$,
- $|E_3(D_3(n))| = 72n^2 - 108n + 44$.


\[
SK(D_3(n)) = \sum_{uv \in E(D_3(n))} \frac{d_u + d_v}{2} = |E_1(D_3(n))| \left( \frac{2 + 2}{2} \right) + |E_2(D_3(n))| \left( \frac{2 + 4}{2} \right) + |E_3(D_3(n))| \left( \frac{4 + 4}{2} \right)
\]

\[
= \frac{4n(2^2)}{2} + \frac{36n^2 - 20n(6 + 4)}{2} + \frac{72n^2 - 108n + 44(8 + 8)}{2}
\]

\[
= 8n + 18n^2 - 10n + 88n^2 - 104n + 352
\]

\[
= 2552n^2 - 2775n + 1015.
\]
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Now,

\[
\chi(D_3(n)) = \sum_{uv \in E(D_3(n))} \frac{1}{\sqrt{d_u + d_v}}
\]

\[
= |E_1(D_3(n))| \frac{1}{\sqrt{2 + 2}} + |E_2(D_3(n))| \frac{1}{\sqrt{2 + 4}} + |E_3(D_3(n))| \frac{1}{\sqrt{2 + 6}}
\]

\[
= \frac{4n}{\sqrt{2}} + \frac{36n^2 - 20n}{\sqrt{6}} + \frac{72n^2 - 108n + 44}{\sqrt{8}}
\]

\[
= (6\sqrt{6} + 18\sqrt{2}) n^2 - \frac{64\sqrt{2}}{100} n + 11\sqrt{2}.
\]

\[
R'(D_3(n)) = \sum_{uv \in E(D_3(n))} \frac{1}{\max\{d_u, d_v\}}
\]

\[
= |E_1(D_3(n))| \frac{1}{\max\{2, 2\}} + |E_2(D_3(n))| \frac{1}{\max\{2, 4\}} + |E_3(D_3(n))| \frac{1}{\max\{2, 6\}}
\]

\[
= \frac{4n}{2} + \frac{36n^2 - 20n}{4} + \frac{72n^2 - 108n + 44}{6}
\]

\[
= 27n^2 - 30n + 11.
\]

\[
AG_1(D_3(n)) = \sum_{uv \in E(D_3(n))} \frac{d_u + d_v}{2 \sqrt{d_u d_v}}
\]

\[
= |E_1(D_3(n))| \frac{2n^2}{2 \sqrt{2}} + |E_2(D_3(n))| \frac{2 + 4}{2 \sqrt{4}} + |E_3(D_3(n))| \frac{2 + 6}{2 \sqrt{6}}
\]

\[
= 4n + (36n^2 - 20n) \left( \frac{6}{\sqrt{6}} \right) + (72n^2 - 108n + 44) \left( \frac{6}{\sqrt{8}} \right)
\]

\[
= (72 + 27\sqrt{2}) n^2 - \frac{132n}{8} n + 44.
\]

\[
SK(D_3(n)) = \sum_{uv \in E(D_3(n))} \frac{d_u d_v}{2}
\]

\[
= |E_1(D_3(n))| \frac{2n}{2} + |E_2(D_3(n))| \frac{2 + 4}{2} + |E_3(D_3(n))| \frac{2 + 6}{2}
\]

\[
= 4n + (36n^2 - 20n) \left( \frac{8}{7} \right) + (72n^2 - 108n + 44) (8)
\]

\[
= 720n^2 - 936n + 352.
\]
3 Graphical comparison

In this section we give graphical comparison of our results Figures 4–9. Turquoise color is for dominating David derived networks of first type, lime color is for dominating David derived network of second type and purple color is for dominating David derived network of third type.

4 Conclusions

In the present report, we computed seven degree-based topological indices of dominating David derived networks of first, second and third type. We compare our results geometrically by plotting computed degree-based indices. We believe that our results play a vital role in preparation of new drugs.

Conflict of Interest:
The authors declare that there is no conflict of interest regarding the publication of this paper.

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