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Biochemical and phylogenetic networks-II: *X*-trees and phylogenetic trees

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Abstract

The present study, which is a continuation of the previous paper, augments a recent work on the use of phylogenetic networks. We develop techniques to characterize the topology of various X-trees and binary trees of biological and phylogenetic interests. We have obtained the results for various *k*-level *X*-trees and phylogenetic networks with variants of Zagreb, Szeged, Padmakar-Ivan, Schultz and Atom Bond Connectivity topological indices.

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1 Introduction

The present study on topological characterization of *X*-trees and binary trees of interest in biological and phylogenetic networks is a continuation of the previous paper by the current authors [1] hereafter to be referred as Paper I. The present work is also stimulated by a recent work of Forster et al. [2] who have outlined the value of phylogenetic network in the context of ongoing coronavirus 2019 (COVID-19) epidemic that has plagued the entire world. They have shown that the graph theoretical network can be utilized in the analysis of virological data, that is, to trace various the COVID-19 sources and to develop mitigation strategies to prevent the spread of the disease. Moreover, such biological networks can also be of great use in machine learning and artificial intelligence applications of controlling the spread of the epidemic through contact tracing, clustering, source identifications and statistical analysis of the epidemic. Such tools can be of great value for efficient identification of the affected persons and subsequent quarantining strategies to facilitate control and spread of the disease. In yet another previous application, Balasubramanian et al. [3] have applied graph theoretical techniques to quantify perturbations of proteomes, for example, the proteomes of rats through externally applied toxins. The resulting proteomic maps or zig-zag trees of amino acids constitute certain topological patterns which alter when external chemicals act on the proteome. Graph theoretical tools have been quite powerful in such biochemical characterizations [3]. Moreover, it has been shown by Balasubramanian [4–7] that tree pruning and other efficient topological techniques can be applied to characterize various trees such as phylogenetic trees, Cayley trees, and Bethe lattices through graph theoretical entities including their characteristic polynomials, symmetries, entropies, and combinatorics of colorings of such trees. Moreover, such recursive and binary trees could be related to recursive relations in molecular shape analysis and recursive generation of Boolean hypercubes that have been considered elsewhere [8–10]. Consequently, there are several biological and biochemical applications of variations of phylogenetic trees such as *X*-trees. For example, in a scenario where there are interactions among certain vertices at a given level of the binary trees, one can model such interactions through the use of *X*-trees that are considered here. These added edges or removed edges from the parent trees could then represent certain biochemical perturbations as described in the context of proteomic maps [3] or in quantifying the effect of added interactions or an infected individual to an infection-free group in an epidemiological study or in quantifying toxicological responses and toxicity profiles.

As pointed out by Forster et al. [2] the phylogenetic network that they constructed using 160 SARS-COV2 genomes, facilitated the evolution of the COVID-19 virus in different regions of the world and its relationship to the assumed source from the bat. Hence they were able to characterize the phylogenetic trees and facilitate delineation into different regions of the world in order to characterize various mutations through the evaluation of the virus in different regions of the world. Such detailed graph theoretical pictures can facilitate

tracing infection pathways as well as mutation pathways for the virus so that one could come up with mitigation strategies. Control strategies for the spread of infectious diseases can be designed by mathematical modelling in epidemiology [11–14]. In the case of epidemic diseases such as COVID-19, an individual infected with the virus turns out to be the root cause of spreading it to a group of disease-free individuals in his neighbourhood. This invasion process affects a large population due to the contacts between this group of infectious individuals and a huge susceptible pool of individuals. In this way, these microorganisms imitate by parting themselves on human bodies, and subsequently ascend to the tree based structures in scientific displaying [15]. Graph theoretical analysis can facilitate detection of root node and intermediate nodes that affect the topology of the network, depending on the epidemic [16]. Consequently, several investigators have considered applications of network theory for a variety of such infections [17–19]. Several topological indices including eccentric index have been developed and applied to characterize such systems [20] as such indices are invariant to labelling of vertices or edges. In the current Paper II, we obtain various topological indices including the eccentricity indices for phylogenetic and *X*-trees that were not considered in Paper I.

All mathematical preliminaries and definitions have been introduced in the accompanying Paper I. Hence readers are referred to Paper I for definitions and preliminaries [1].

2 Results and discussion

An *X*-tree $XT(l)$ is obtained from the complete binary tree T_l on $2^{l+1} - 1$ vertices, and joining all the vertices in each level i from left to right, $1 \leq i \leq l$. The graph $XT(4)$ is given in Fig. 1.
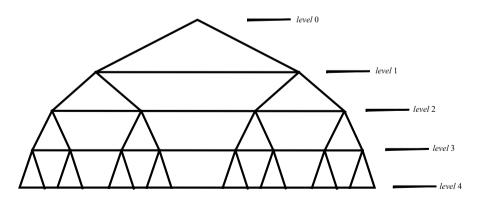

Fig. 1 The *X*-tree network $XT(4)$

Table 1 Results obtained for *l*-level *X*-tree network *XT*(*l*), with the computer code compared with the results from the expressions derived here and those from Ref. [21]

Index	Dimension *l*	TopoChemie-2020	From expressions 2.1	Ref. [21]
GA_4	$l=3$	24.880794488885737	24.8807	28.8397
	$l=4$	55.86286296173727	55.8629	105.6604
	$l=5$	118.83638101813052	118.8363	316.4091
	$l=6$	245.79225807606497	245.7922	837.0146
Zg_4	$l=3$	190	190	218
	$l=4$	626	626	1126
	$l=5$	1776	1776	4344
	$l=6$	4616	4616	14,058
Π_4^*	$l=3$	7.318411747025515E+21	7.3184E+21	78,382,080
	$l=4$	2.2951471834362743E+58	2.2952E+58	2.51612254E21
	$l=5$	1.1636771331250612E+139	1.1637E+139	4.39862658E46
	$l=6$	+Inf	+Inf	1.43477106E87
Zg_6	$l=3$	368	368	416
	$l=4$	1789	1789	3042
	$l=5$	6757	6757	15,177
	$l=6$	22,002	22,002	60,158
Π_6^*	$l=3$	3.7439062426244873E+28	3.7439e+28	2,239,488,000
	$l=4$	7.706715809924782E+82	7.7067e+82	1.17568345E26
	$l=5$	2.2091018217754644E+206	2.2092e+206	5.52706905E57
	$l=6$	+Inf	+Inf	4.1859e+107
$ABC_5\Pi$	$l=3$	0.000008336974857890423	8.3426e-06	228.5933044733
	$l=4$	1.7793072547793842E-15	1.7330e-15	17,723,692.8320256
	$l=5$	3.384275421412989E-38	3.3876e-38	3.84834506E16
	$l=6$	7.635281023554304E-89	7.6237e-89	7.19232813E31

We have previously pointed out in Paper I [1] errors made by Gao et al. [21] in the computations of various topological indices and enumerated various steps in pointing out the errors. Table 1 shows all of the indices for the *X*-trees that we have obtained in the present work by correcting the previous results of Gao et al. [21] and the results computed from TopoChemie-2020 [22], a suite of Fortran'95 codes to compute all of the topological indices.

The corrected Theorem 2.1 for the topological indices follows.

Theorem 2.1 (Corrected Theorem 2 of [21]) *Let $XT(l)$ be the $l-$ level X-tree with $l \geq 3$. Then we have the following:*

$$GA_4(XT(l)) = 2^{l+1} - 3l + 4 + 2\sum_{a=1}^{l-2}(3 \times 2^a + 2)\frac{\sqrt{(l+a-1)(l+a)}}{2(l+a)-1}$$

$$+ 2(2^{l-1}+2)\frac{\sqrt{(2l-2)(2l-1)}}{4l-3};$$

$$Zg_4(XT(l)) = 16l \times 2^l - 22 \times 2^l - 3l^2 - 7l + 30;$$

$$\Pi_4^*(XT(l)) = 64l^6 \times \prod_{a=1}^{l-2}(2(l+a))^{3 \cdot 2^a - 3} \times \prod_{a=1}^{l-2}(2(l+a)-1)^{3 \cdot 2^a + 2} \times (4l-3)^{2^{l-1}+2}$$

$$\times (4l-2)^{2^{l-1}-2};$$

$$Zg_6(XT(l)) = \frac{173l}{6} + 44l \times 2^l + 39 \times 2^l - \frac{5l^2}{2} - \frac{7l^3}{3} + 16l^2 \times 2^l - 41;$$

$$\Pi_6^*(XT(l)) = l^{12} \times \prod_{a=1}^{l-2}(l+a)^{6(2^a-1)} \times \prod_{a=1}^{l-2}((l+a-1)(l+a))^{3 \cdot 2^a + 2}$$

$$\times \left(4l^2 - 6l + 2\right)^{(2^{l-1}+2)} \times (2l-1)^{2(2^{l-1}-2)};$$

$$Zg_4(XT(l), x) = \sum_{a=1}^{l-2}3(2^a - 1)x^{2(l+a)} + \sum_{a=1}^{l-2}(3 \times 2^a + 2)x^{2(l+a)-1}$$

$$+ (2^{l-1}+2)x^{4l-3} + (2^{l-1}-2)x^{4l-2} + 6x^{2l};$$

$$Zg_6(XT(l), x) = \sum_{a=1}^{l-2}3(2^a - 1)x^{(l+a)^2} + \sum_{a=1}^{l-2}(3 \times 2^a + 2)x^{(l+a-1)(l+a)}$$

$$+ (2^{l-1}+2)x^{(2l-2)(2l-1)} + (2^{l-1}-2)x^{(2l-1)^2} + 6x^{l^2};$$

$$ABC_5\Pi(XT(l)) = \prod_{a=1}^{l-2}\left(\frac{\sqrt{2(l+a)-2}}{(l+a)}\right)^{3(2^a - 1)} \times \prod_{a=1}^{l-1}\left(\frac{2(l+a)-3}{(l+a-1)(l+a)}\right)^{3 \cdot 2^{a-1}+1}$$

$$\times \left(\frac{4l-5}{(2l-2)(2l-1)}\right)^{2^{l-2}+1} \times \left(\frac{2\sqrt{l-1}}{2l-1}\right)^{2^{l-1}-2} \times \left(\frac{\sqrt{2l-2}}{l}\right)^6.$$

Proof First, we partition the edge set of $XT(l)$ as follows:

- $E_{ll} = \{e = st \in E(XT(l)) | \eta(s) = \eta(t) = l\}$; $n_{ll} = |E_{ll}| = 6$;
- $E_{(l+a)(l+a)} = \{e = st \in E(XT(l)) | \eta(s) = \eta(t) = l+a\}$; $n_{(l+a)(l+a)}$ $= |E_{(l+a)(l+a)}| = 3 \cdot 2^a - 3$, where $a \in [l-2]$;
- $E_{(l+a-1)(l+a)} = \{e = st \in E(XT(l)) | \eta(s) = l+a-1$ and $\eta(t) = l+a\}$ and $n_{(l+a-1)(l+a)} = |E_{(l+a-1)(l+a)}| = 3(2^a) + 2$, where $a \in [l-2]$;

- $E_{(2l-2)(2l-1)} = \{e = st \in E(XT(l)) | \eta(s) = 2l - 2 \text{ and } \eta(t) = 2l - 1\}$ and
  $n_{(2l-2)(2l-1)} = \left| E_{(2l-2)(2l-1)} \right| = 2(2^{l-2}) + 2;$

- $E_{(2l-1)(2l-1)} = \{e = st \in E(XT(l)) | \eta(s) = \eta(t) = 2l - 1\}$ and $n_{(2l-1)(2l-1)} =$
  $\left| E_{(2l-1)(2l-1)} \right| = 2(2^{l-2}) - 2,$ where $a = l - 2.$

By the definition, we have

$$GA_4(XT(l)) = 6 + \sum_{a=1}^{l-2}(3 \cdot 2^a - 3) + \sum_{a=1}^{l-2}(3 \cdot 2^a + 2)\left(\frac{2\sqrt{(l+a-1)(l+a)}}{2l+2a-1}\right)$$

$$+ \left(2 \cdot 2^{l-2} + 2\right)\frac{2\sqrt{(2l-2)(2l-1)}}{4l-3} + \left(2 \cdot 2^{l-2} - 2\right)$$

$$= 2^{l+1} - 3l + 4 + 2\sum_{a=1}^{l-2}(3 \times 2^a + 2)\frac{\sqrt{(l+a-1)(l+a)}}{2(l+a)-1}$$

$$+ 2\left(2^{l-1} + 2\right)\frac{\sqrt{(2l-2)(2l-1)}}{4l-3};$$

$$Zg_4(XT(l)) = 12l + \sum_{a=1}^{l-2}(3 \cdot 2^a - 3).2.(l+a)$$

$$+ \sum_{a=1}^{l-2}(3 \cdot 2^a + 2)(2l + 2a - 1) + \left(2 \cdot 2^{l-2} + 2\right)(4l - 3)$$

$$+ \left(2 \cdot 2^{l-2} - 2\right)(4l - 2)$$

$$= 16l \times 2^l - 22 \times 2^l - 3l^2 - 7l + 30;$$

$$\Pi_4^*(XT(l)) = (2l)^6 \times \prod_{a=1}^{l-2}(2(l+a))^{(3 \cdot 2^a - 3)} \times \prod_{a=1}^{l-2}(2(l+a) - 1)^{(3 \cdot 2^a + 2)}$$

$$\times (4l - 3)^{(2 \cdot 2^{l-2} + 2)} \times (4l - 2)^{(2 \cdot 2^{l-2} - 2)}$$

$$= 64l^6 \times \prod_{a=1}^{l-2}(2(l+a))^{3 \cdot 2^a - 3} \times \prod_{a=1}^{l-2}(2(l+a) - 1)^{3 \cdot 2^a + 2}$$

$$\times (4l - 3)^{2^{l-1} + 2} \times (4l - 2)^{2^{l-1} - 2};$$

$$Zg_6(XT(l)) = 6l^2 + \sum_{a=1}^{l-2}(3 \cdot 2^a - 3).(l+a)^2$$

$$+ \sum_{a=1}^{l-2}(3 \cdot 2^a + 2)(l + a - 1)(l + a)$$

$$+ \left(2 \cdot 2^{l-2} + 2\right)(2l - 2)(2l - 1) + \left(2 \cdot 2^{l-2} - 2\right)(2l - 1)(2l - 1)$$

$$= \frac{173l}{6} + 44l \times 2^l + 39 \times 2^l - \frac{5l^2}{2} - \frac{7l^3}{3} + 16l^2 \times 2^l - 41;$$

Proceeding along the same lines, we prove the remaining equations.

3 Certain distance and degree based topological indices of *X*-trees and phylogenetic trees.

In this section, we compute certain distance and degree based topological indices of *X*-tree, and phylogenetic trees that have not been obtained earlier.

3.1 *X*-tree network

In this section, we compute the first Zagreb, second Zagreb, and atom bond connectivity index of the *l*-level *X*-tree network $XT(l), l \geq 2$.

Theorem 3.1.1 *Let $XT(l), l \geq 2$ be the l-level X-tree network. Then the first Zagreb index,*

$$M_1(XT(l)) = 34 \times 2^l - 18l - 38.$$

Proof First, we partition the vertex set of $XT(l)$ as follows:

$$P_1 = \{v | d(v) = 2\} \text{ and } |P_1| = 3.$$
$$P_2 = \{v | d(v) = 3\} \text{ and } |P_2| = 2^l - 2.$$
$$P_3 = \{v | d(v) = 4\} \text{ and } |P_3| = 2(l - 1).$$
$$P_4 = \{v | d(v) = 5\} \text{ and } |P_4| = 2^{l+1} - 2^l - 2l.$$

By the definition, we have

$$
\begin{aligned}
M_1(XT(l)) &= (3)2^2 + \left(2^l - 2\right)3^2 + (2(l-1))4^2 + (2^{l+1} - 2^l - 2l)5^2 \\
&= 34 \times 2^l - 18l - 38.
\end{aligned}
$$

Theorem 3.1.2 *Let $XT(l), l \geq 2$ be the l-level X-tree network. Then the atom bond connectivity index*

$$ABC(XT(l)) = 1.2991221987(2^l) + 0.56568542495(2^{l+1}) - 0.36862119001(l) - 2.17205557615.$$

Proof First, we partition the edge set of $XT(l)$ as follows:

$E_{23} = \{e = uv \in E(XT(l)) | d(u) = 2 \text{ and } d(v) = 3\} \text{ and } |E_{23}| = 1.$

$E_{24} = \{e = uv \in E(XT(l)) | d(u) = 2 \text{ and } d(v) = 4\} \text{ and } |E_{24}| = 2.$

$E_{32} = \{e = uv \in E(XT(l)) | d(u) = 3 \text{ and } d(v) = 2\} \text{ and } |E_{32}| = 1.$

$E_{33} = \{e = uv \in E(XT(l)) | d(u) = 3 \text{ and } d(v) = 3\} \text{ and } |E_{33}| = 2^l - 3.$

$E_{42} = \{e = uv \in E(XT(l)) | d(u) = 4 \text{ and } d(v) = 2\} \text{ and } |E_{42}| = 2.$

$E_{43} = \{e = uv \in E(XT(l)) | d(u) = 4 \text{ and } d(v) = 3\} \text{ and } |E_{43}| = 2.$

$E_{44} = \{e = uv \in E(XT(l)) | d(u) = 4 \text{ and } d(v) = 4\} \text{ and } |E_{44}| = 2l - 3.$

$E_{45} = \{e = uv \in E(XT(l)) | d(u) = 4 \text{ and } d(v) = 5\} \text{ and } |E_{45}| = 3l - 6.$

$E_{53} = \{e = uv \in E(XT(l)) | d(u) = 5 \text{ and } d(v) = 3\} \text{ and } |E_{53}| = 2^l - 4.$

$E_{54} = \{e = uv \in E(XT(l)) | d(u) = 5 \text{ and } d(v) = 4\} \text{ and } |E_{54}| = l - 2.$

$E_{55} = \{e = uv \in E(XT(l)) | d(u) = 5 \text{ and } d(v) = 5\} \text{ and } |E_{55}| = 2^{l+1} - 7l + 6.$

By the definition, we have

$$ABC(XT(l)) = \sum_{e \in E_{23}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{24}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{32}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$+ \sum_{e \in E_{33}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{42}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{43}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$+ \sum_{e \in E_{44}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{45}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$+ \sum_{e \in E_{53}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{54}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$+ \sum_{e \in E_{55}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} = 1\sqrt{\frac{1}{2}} + 2\sqrt{\frac{1}{2}} + 1\sqrt{\frac{1}{2}} + (2^l - 3)\left(\frac{2}{3}\right)$$

$$+ 2\sqrt{\frac{1}{2}} + 2\sqrt{\frac{5}{12}} + (2l - 3)\sqrt{\frac{3}{8}} + (3l - 6)\sqrt{\frac{7}{20}}$$

$$+ (2^l - 4)\sqrt{\frac{6}{15}} + (l - 2)\sqrt{\frac{7}{20}} + (2^{l+1} - 7l + 6)\sqrt{\frac{8}{25}}$$

$$= 1.2991221987\,(2^l) + 0.56568542495(2^{l+1}) - 0.36862119001\,(l) - 2.17205557615.$$

Theorem 3.1.3 *Let $XT(l), l \geq 2$ be the X-tree network of l-level. Then the second Zagreb index $M_2(XT(l)) = 25 \times 2^{l+1} - 63 \times l + 24 \times 2^l - 77$.*

The proof runs analogous to that of Theorem 3.1.2.

Theorem 3.1.4 *Let $XT(l), l \geq 2$ be the l-level X-tree network. Then the PI index*

$$PI(XT(l)) = 2^{2l+2} + 2^l[4l^2 - 18l + 16] + 4l^2 + 2l - 20.$$

Proof Let $\quad A = \{e = uv | u \text{ in level } i \text{ and } v \text{ in level } i+1, 0 \leq i \leq l-1\}, \; B = \{e = uv | u \text{ and } v \text{ in the same level } i, 1 \leq i \leq l\}$, and let j be the position of the edge from left most edge to right most edge in level i.

Case (i): $e \in A$

If $i = 0$, then it is easy to verify that $n(u) = 1$ and $n(v) = 2^l - 1$. Thus

$$n(u) + n(v) = 2^l \tag{1}$$

For any $i, j, 1 \leq i \leq l-1,$ and $3 \leq j \leq 2^i - 1, n(u) = 2(2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 6(2^{l-i} - 1)$. Thus,

$$n(u) + n(v) = (2^{l+1} - 1) - 4(2^{l-i} - 1) \tag{2}$$

For any $i, j, 1 \leq i \leq l-1,$ and $j = 1, n(u) = (2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 3(2^{l-i} - 1)$. Thus

$$n(u) + n(v) = (2^{l+1} - 1) - 2(2^{l-i} - 1) \tag{3}$$

For any $i, j, 1 \leq i \leq l-1$, and $j = 2^i$ or 2, $n(u) = 2(2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 5(2^{l-i} - 1)$. Thus

$$n(u) + n(v) = (2^{l+1} - 1) - 3(2^{l-i} - 1) \tag{4}$$

Hence by Eqs. (1)–(3), and (4), we get

$$PI_1(XT(l)) = 2\left[2^l + \sum_{j=3}^{2^i-1}[(2^{l+1} - 1) - 4(2^{l-i} - 1)] + (2^{l+1} - 1) - 2(2^{l-i} - 1) + 2((2^{l+1} - 1) - 3(2^{l-i} - 1))\right]$$

$$= 2^{l+1} + 2^l[2^{l+2} - 8l + 14] - 8l - 20 \tag{I}$$

Case (ii): $e \in B$

If $i = 1$, then it is easy to verify that $n(u) = n(v) = 2^l - 1$. Further there are l similar edges in the edge subset E_l such that $n(u) = n(v) = 2^l - 1$. Thus

$$\sum_{uv \in E_l} (n(u) + n(v)) = l(2^{l+1} - 2) \tag{5}$$

If $i = 2$, then $n(u) = \left(2^{l-1} - 1\right)$ and $n(v) = 2^{l+1} - 2^{l-1} - 3$. Then $n(u) + n(v) = 2^{l+1} - 4$. Further there are $l - 1$ similar edges in the subset E_{l-1} such that $n(u) + n(v) = 2^{l+1} - 4$. Thus

$$\sum_{uv \in E_{l-1}} (n(u) + n(v)) = (l - 1)(2^{l+1} - 4) \tag{6}$$

For any $i, j, 3 \le i \le l$, and $3 \le j \le 2^{i-2}, n(u) = n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in the subset E_{l-i+1} such that $n(u) = n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) + n(v)) = (l - i + 1) \times 8 \times \left(2^{l-i+1} - 1\right) \tag{7}$$

For any $i, j, 3 \le i \le l$, and $j = 1$, $n(u) = \left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in the subset E_{l-i+1} such that $n(u) = \left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) + n(v)) = (l - i + 1) \times 5 \times \left(2^{l-i+1} - 1\right) \tag{8}$$

For any $i, j, 3 \le i \le l$, and $j = 2$, $n(u) = 3\left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in E_{l-i+1} such that $n(u) = 3\left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) + n(v)) = (l - i + 1) \times 7 \times \left(2^{l-i+1} - 1\right) \tag{9}$$

Hence by Eqs. (5)–(8) and (9), we get

$$PI_2(XT(l)) = l(2^{l+1} - 2) + 2\left[(l - 1)\left(2^{l+1} - 4\right)\right]$$
$$+ 2\sum_{i=3}^{l}\left[\left(\sum_{j=3}^{2^{i-2}}(l - i + 1) \times 8 \times \left(2^{l-i+1} - 1\right)\right) + (l - i + 1)\right.$$
$$\left. \times 5 \times \left(2^{l-i+1} - 1\right) + (l - i + 1) \times 7 \times \left(2^{l-i+1} - 1\right)\right]$$
$$= 2l\left(2l + 2l \times 2^l - 5 \times 2^l + 5\right) \tag{II}$$

From (I) and (II), we have

$$PI(XT(l)) = PI_1(XT(l)) + PI_2(XT(l))$$
$$= 2^{2l+2} + 2^l\left[4l^2 - 18l + 16\right] + 4l^2 + 2l - 20.$$

Theorem 3.1.5 *Let $XT(l), l \geq 2$ be the l-level X-tree network. Then the Szeged index*

$$Sz(XT(l)) = 8 \times 2^l \times l - \frac{775 \times 2^{2l}}{18} - 17l + 58 \times 2^l + 16 \times l^2 + \frac{79 \times 2^{2l} \times l}{6}$$

$$- \frac{76}{9} + 2\sum_{i=3}^{l}(l - i + 1) \times 16 \times \left(2^{l-i+1} - 1\right)^2 \times \left(2^{i-2} - 2\right)$$

Proof Let $A = \{e = uv | u \text{ in level } i \text{ and } v \text{ in level } i+1, 0 \leq i \leq l-1\}$, $B = \{e = uv | u \text{ and } v \text{ in the same level } i, 1 \leq i \leq l\}$, *and* j *be the position of the edge from left most edge to right most edge in level* i.

Case (i): $e \in A$

If $i = 0$, then it is easy to verify that $n(u) = 1$ and $n(v) = 2^l - 1$. Thus

$$n(u) \times n(v) = 2^l - 1 \tag{10}$$

For any $i, j, 1 \leq i \leq l-1$, and $3 \leq j \leq 2^i - 1$, $n(u) = 2(2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 6(2^{l-i} - 1)$. Thus

$$n(u) \times n(v) = (2 \times 2^{l-i} - 2)(2^{l+1} - 6 \times 2^{l-i} + 5) \tag{11}$$

For any $i, j, 1 \leq i \leq l-1$, and $j = 1$, $n(u) = (2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 3(2^{l-i} - 1)$. Thus

$$n(u) \times n(v) = (2^{l-i} - 1)(2^{l+1} - 3 \times 2^{l-i} + 2) \tag{12}$$

For any $i, j, 1 \leq i \leq l-1$, and $j = 2^i$ *or* 2, $n(u) = 2(2^{l-i} - 1)$ and $n(v) = (2^{l+1} - 1) - 5(2^{l-i} - 1)$. Consequently,

$$n(u) \times n(v) = (2 \times 2^{l-i} - 2)(2^{l+1} - 5 \times 2^{l-i} + 4) \tag{13}$$

Hence by Eqs. (10)–(12), and (13), we get

$$Sz_1(XT(l)) = 2\left[\left(2^l - 1\right) + \sum_{j=3}^{2^i-1}\left[\left(2 \times 2^{l-i} - 2\right)\left(2^{l+1} - 6 \times 2^{l-i} + 5\right)\right]\right.$$
$$\left. + \left(2^{l-i} - 1\right)\left(2^{l+1} - 3 \times 2^{l-i} + 2\right) + 2\left(\left(2 \times 2^{l-i} - 2\right)\left(2^{l+1} - 5 \times 2^{l-i} + 4\right)\right)\right]$$
$$= 24l - \frac{106 \times 2^{2l}}{3} + 48 \times 2^l \times l - 44 \times 2^l + 8 \times 2^{2l} \times l + \frac{238}{3} \tag{III}$$

Case (ii): $e \in B$

If $i = 1$, then it is easy to verify that $n(u) = n(v) = 2^l - 1$. Further there are l similar edges in E_1 such that $n(u) = n(v) = 2^l - 1$. Thus

$$\sum_{uv \in E_l} (n(u) \times n(v)) = l(2^l - 1)^2 \tag{14}$$

If $i = 2$, then $n(u) = \left(2^{l-1} - 1\right)$ and $n(v) = 2^{l+1} - 2^{l-1} - 3$. Then $n(u) \times n(v) = \left(2^{l-1} - 1\right) \times (2^{l+1} - 2^{l-1} - 3)$. Further there are $l - 1$ similar edges in E_{l-1} such that $n(u) \times n(v) = \left(2^{l-1} - 1\right) \times (2^{l+1} - 2^{l-1} - 3)$. Thus

$$\sum_{uv \in E_{l-1}} (n(u) \times n(v)) = (l - 1) \times \left(2^{l-1} - 1\right) \times (2^{l+1} - 2^{l-1} - 3) \tag{15}$$

For any $i, j, 3 \leq i \leq l$, and $3 \leq j \leq 2^{i-2}$, $n(u) = n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in E_{l-i+1} such that $n(u) = n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) \times n(v)) = (l - i + 1) \times (16) \times \left(2^{l-i+1} - 1\right)^2 \tag{16}$$

For any $i, j, 3 \leq i \leq l$, and $j = 1$, $n(u) = \left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in E_{l-i+1} such that $n(u) = \left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) \times n(v)) = (l - i + 1) \times \left(2^{l-i+1} - 1\right) \times 4\left(2^{l-i+1} - 1\right) \tag{17}$$
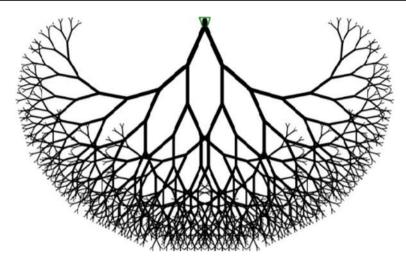
Table 2 Results obtained for the l-level X-tree network $XT(l)$ with the computer code compared with the results from the expressions in Theorems 3.1.1–3.1.5

Index	Dimension l	TopoChemie-2020	From expressions 3.1.1–3.1.5
$ABC(XT(l))$	$l=3$	16.16602524259959	16.16602524262
	$l=4$	35.2413484413769	35.24134844141
	$l=5$	73.76061602894474	73.760616029
	$l=6$	151.1677723940934	151.16777239419
$M_1(XT(l))$	$l=3$	180	180
	$l=4$	434	434
	$l=5$	960	960
	$l=6$	2030	2030
$M_2(XT(l))$	$l=3$	326	326
	$l=4$	855	855
	$l=5$	1976	1976
	$l=6$	4281	4281
$PI(XT(l))$	$l=3$	262	262
	$l=4$	1204	1204
	$l=5$	5018	5018
	$l=6$	19,848	19,848
$Sz(XT(l))$	$l=3$	513	513
	$l=4$	4144	4144
	$l=5$	28,111	28,111
	$l=6$	167,790	167,790

For any $i, j, 3 \leq i \leq l$, and $j = 2$, $n(u) = 3\left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Further there are $(l - i + 1)$ similar edges in E_{l-i+1} such that $n(u) = 3\left(2^{l-i+1} - 1\right)$ and $n(v) = 4\left(2^{l-i+1} - 1\right)$. Thus

$$\sum_{uv \in E_{l-i+1}} (n(u) \times n(v)) = (l - i + 1) \times 3 \times \left(2^{l-i+1} - 1\right) \times 4 \times \left(2^{l-i+1} - 1\right) \quad (18)$$

Hence by Eqs. (14)–(17) and (18), we get

$$Sz_2(XT(l)) = l(2^l - 1)^2 + 2[(l - 1) \times (2^{l-1} - 1) \times (2^{l+1} - 2^{l-1} - 3)]$$

$$+ 2\left[\sum_{i=3}^{l}\left[\sum_{i=3}^{2^{i-2}}[(l - i + 1) \times (16) \times (2^{l-i+1} - 1)^2]\right] + (l - i + 1)\right.$$

$$\left. \times (2^{l-i+1} - 1) \times 4(2^{l-i+1} - 1) + (l - i + 1) \times 3 \times (2^{l-i+1} - 1) \times 4 \times (2^{l-i+1} - 1)\right]$$

$$= 102 \times 2^l - \frac{139 \times 2^{2l}}{18} - 40 \times 2^l \times l - 41 \times l + 16 \times l^2 + \frac{31 \times 2^{2l} \times l}{6} - \frac{790}{9}$$

$$+ 2\sum_{i=3}^{l}(l - i + 1) \times 16 \times \left(2^{l-i+1} - 1\right)^2 \times \left(2^{i-2} - 2\right) \quad \text{(IV)}$$

Fig. 2 The complete binary (2-ary) tree T_{10}^2 of level 10

From (III) and (IV), we have

$$Sz(XT(l)) = Sz_1(XT(l)) + Sz_2(XT(l))$$

$$= 8 \times 2^l \times l - \frac{775 \times 2^{2l}}{18} - 17l + 58 \times 2^l + 16 \times l^2 + \frac{79 \times 2^{2l} \times l}{6} - \frac{76}{9}$$

$$+ 2 \sum_{i=3}^{l} (l - i + 1) \times 16 \times \left(2^{l-i+1} - 1\right)^2 \times \left(2^{i-2} - 2\right).$$

Remark 3.1.6 The results obtained from TopoChemie-2020 are shown in Table 2 for comparison with the results obtained from Theorems 3.1.1–3.1.5.

3.2 Phylogenetic tree network

For any non-negative integer l, the complete k-ary tree of level l, denoted by T_l^k, is the k-ary tree (a tree in which each node has no more than k children), where each internal vertex has exactly k children and all the leaves are at the same level. Clearly, a complete k-ary tree T_l^k has l levels and level i, $0 \leq i \leq l$ contains k^i vertices. Thus T_l^k has exactly $\frac{k^{l+1}-1}{k-1}$ vertices. The complete k-ary tree when all vertices have the same degree (except terminal vertices)is also called as Cayley tree network

or phylogenetic tree networks. For illustration the complete binary (2-ary) tree of level 10, T_{10}^2 is given in Fig. 2. In this section, we consider complete binary tree T_l^2 of level l for further studies and denote it as T_l.

Theorem 3.2.1 *Let T_l be the complete binary tree network, $l \geq 2$. Then the atom bond connectivity index*

$$ABC(T_l) = 2\sqrt{\frac{3}{6}} + 2^l\sqrt{\frac{2}{3}} + (2^l - 2^2).\frac{\sqrt{4}}{3}$$

Proof First, we partition the edge set of T_l as follows:

$$E_{23} = \{e = uv \in E(T_l) | d(u) = 2 \text{ and } d(v) = 3\} \text{ and } |E_{23}| = 2.$$
$$E_{13} = \{e = uv \in E(T_l) | d(u) = 1 \text{ and } d(v) = 3\} \text{ and } |E_{13}| = 2^l.$$
$$E_{33} = \{e = uv \in E(T_l) | d(u) = 3 \text{ and } d(v) = 3\} \text{ and } |E_{33}| = \sum_{i=2}^{l-1} 2^i.$$

By the definition, we have

$$\begin{aligned}
ABC(T_l) &= \sum_{e \in E_{23}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{e \in E_{13}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} \\
&\quad + \sum_{e \in E_{33}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} \\
&= 2\sqrt{\frac{3}{6}} + 2^l\sqrt{\frac{2}{3}} + (2^l - 2^2).\frac{\sqrt{4}}{3}
\end{aligned}$$

Theorem 3.2.2 *Let T_l be the complete binary tree network, $l \geq 2$. Then the first Zagreb index $M_1(T_l) = 10 \times 2^l - 14$.*

Proof First, we partition the vertex set of T_l as follows:

$$P_1 = \{v | d(v) = 2\} \text{ and } |P_1| = 1.$$

$$P_2 = \{v | d(v) = 3\} \text{ and } |P_2| = 2^l - 2.$$

$$P_3 = \{v | d(v) = 1\} \text{ and } |P_3| = 2^l.$$

By the definition, we have

$$\begin{aligned}
M_1(T_l) &= \sum_{v \in P_1} (d(v))^2 + \sum_{v \in P_2} (d(v))^2 + \sum_{v \in P_3} (d(v))^2 \\
&= 4 + 9(2^l - 2) + 2^l \\
&= 10 \times 2^l - 14.
\end{aligned}$$

Theorem 3.2.3 *Let T_l be the complete binary tree network, $l \geq 2$. Then the second Zagreb index $M_2(T_l) = 12 \times 2^l - 24$.*

The proof runs analogous to that of Theorem 3.2.1.

The Szeged index has been extensively studied for a variety of graphs, and in fact Gutman and coworkers [23] have shown that the Szeged index is identical to the celebrated Wiener index for all trees, and thus for the phylogenetic binary trees considered here, the Szeged indices are the same as Wiener indices and the numerical results obtained from TopoChemie-2000 for W and Sz of binary trees confirmed this fact.

Theorem 3.2.4 *Let $T_l, l \geq 2$ be the complete binary tree network of level l. Then the Szeged index*

$$Sz(T_l) = 2^{l+1}(l + l \times 2^{l+1} - 4 \times 2^l + 4).$$

Proof First, we partition the edge set of T_l as follows:

$$E_{23} = \{e = uv \in E(T_l) | d(u) = 2, d(v) = 3, n(u) = (2^l - 1) \text{ and } n(v) = (2^l)\} \text{ and } |E_{23}| = 2.$$

$$E_{13} = \{e = uv \in E(T_l) | d(u) = 1 \text{ and } d(v) = 3, n(u) = 1 \text{ and } n(v) = 2^{l+1} - 2\} \text{ and } |E_{13}| = 2^l.$$

$$E_{33} = \left\{ e = uv \in E(T_l) | d(u) = 3 \text{ and } d(v) = 3, n(u) = \sum_{i=1}^{l-2}(2^{i+1} - 1) \text{ and } \right.$$

$$\left. n(v) = \sum_{i=1}^{l-2}((2^{l+1} - 1) - (2^{i+1} - 1)) \right\} \text{ and } |E_{33}| = \sum_{i=1}^{l-2}(2^{l-i}).$$

By the definition, we have

$$Sz(T_l) = ((2^l - 1) \times 2^l) \times 2 + (1 \times 2^{l+1} - 2) \times 2^l$$

$$+ \sum_{i=1}^{l-2} ((2^{i+1} - 1) \times ((2^{l+1} - 1) - (2^{i+1} - 1)))2^{l-i}$$

$$= 2^{l+1}(l + l \times 2^{l+1} - 4 \times 2^l + 4).$$

Theorem 3.2.5 *Let $T_l, l \geq 2$ be the complete binary tree network of level l. Then the PI index.*

$$PI(T_l) = 4 \times 2^{2l} - 6 \times 2^l + 2$$

Proof First, we partition the edge set of T_l as follows:

$$E_{23} = \{e = uv \in E(T_l) | d(u) = 2, d(v) = 3, n(u) = (2^l - 1) \text{ and } n(v) = (2^l)\} \text{ and } |E_{23}| = 2.$$

$$E_{13} = \{e = uv \in E(T_l) | d(u) = 1 \text{ and } d(v) = 3, n(u) = 1 \text{ and } n(v) = 2^{l+1} - 2\} \text{ and } |E_{13}| = k^l$$

$$E_{33} = \left\{ e = uv \in E(T_l) | d(u) = 3 \text{ and } d(v) = 3, n(u) = \sum_{i=1}^{l-2}(2^{i+1} - 1) \text{ and } \right.$$

$$\left. n(v) = \sum_{i=1}^{l-2}((2^{l+1} - 1) - (2^{i+1} - 1)) \right\} \text{ and } |E_{33}| = \sum_{i=1}^{l-2}(2^{l-i})$$

Table 3 Results obtained for Phylogenetic Network T_l, with the computer code compared with the results from the expressions in Theorems 3.2.1–3.2.7

Index	Dimension l	TopoChemie-2020	From expressions 3.2.1–3.2.7
$ABC(T_l)$	$l=3$	10.612852876461572	10.613
	$l=4$	22.478158857216716	22.478
	$l=5$	46.208770818727004	46.2088
$M_1(T_l)$	$l=3$	66	66
	$l=4$	146	146
	$l=5$	306	306
$M_2(T_l)$	$l=3$	72	72
	$l=4$	168	168
	$l=5$	360	360
$Sz(T_l)$	$l=3$	368	368
	$l=4$	2304	2304
	$l=5$	12,864	12,864
$PI(T_l)$	$l=3$	210	210
	$l=4$	930	930
	$l=5$	3906	3906
$S(T_l)$	$l=3$	1262	1262
	$l=4$	8286	8286
	$l=5$	47,550	47,550
$GUT(T_l)$	$l=3$	1066	1066
	$l=4$	7386	7386
	$l=5$	43,706	43,706

By the definition, we have

$$PI(T_l) = \left((2^l - 1) + 2^l\right) \times 2 + \left(1 + 2^{l+1} - 2\right) \times 2^l$$

$$+ \sum_{i=1}^{l-2} \left((2^{i+1} - 1) + ((2^{l+1} - 1) - (2^{i+1} - 1))\right)2^{l-i}$$

$$= 4 \times 2^{2l} - 6 \times 2^l + 2$$

Theorem 3.2.6 *Let $T_l, l \geq 2$ be the complete binary tree network of level l. Then the Schultz index*

$$S(T_l) = 8l \times 2^l - 36 \times 2^{2l} + 38 \times 2^l + 16l \times 2^{2l} - 2.$$

Proof We partition the vertices (ordered pairs) of T_l as follows:

$$V_{11} = \{(x,y)/d(x) = d(y) = 1\} \text{ and } |V_{11}| = 2^{l-1}(2^l - 1)$$
$$V_{12} = \{(x,y)/d(x) = 1 \text{ and } d(y) = 2\} \text{ and } |V_{12}| = 2^l$$
$$V_{13} = \{(x,y)/d(x) = 1 \text{ and } d(y) = 3\} \text{ and } |V_{13}| = 2^l(2^l - 2)$$
$$V_{23} = \{(x,y)/d(x) = 2 \text{ and } d(y) = 3\} \text{ and } |V_{23}| = (2^l - 2) \text{ and }$$
$$V_{33} = \{(x,y)/d(x) = d(y) = 3\} \text{ and } |V_{33}| = \frac{(2^l - 2)(2^l - 3)}{2}.$$

By the definition, we have

$$
\begin{aligned}
S(T_l) &= \sum_{(u,v)\in V_{11}} (d(u) + d(v))\, d(u,v) + \sum_{(u,v)\in V_{12}} (d(u) + d(v))\, d(u,v) + \sum_{(u,v)\in V_{13}} (d(u) + d(v))\, d(u,v) \\
&\quad + \sum_{(u,v)\in V_{23}} (d(u) + d(v))\, d(u,v) + \sum_{(u,v)\in V_{33}} (d(u) + d(v))\, d(u,v) \\
&= (1 + 1)\left[\left(\sum_{i=1}^{l} 2i \times 2^{i-1}\right)2^{l-1}\right] + (1 + 2)l \times 2^l \\
&\quad + (1 + 3)\left[\sum_{i=2}^{l-1}\sum_{j=1}^{i-1}(l - i + 2j)2^{l+j-1} + \sum_{i=1}^{l-1}(l - i)2^l + \sum_{i=1}^{l-1}(l + i)2^{l+i-1}\right] \\
&\quad + (2 + 3)\left[\sum_{i=1}^{l-1} i \times 2^i\right] + (3 + 3)\left[\sum_{k=1}^{l-2}\left[\sum_{i=2}^{l-1-k}\left(\sum_{j=1}^{i-1}(l - i + 2j - k)2^{l+j-k-1}\right)\right] + \sum_{k=1}^{l-2}\left(\sum_{i=1}^{l-1-k}(l - i - k)2^{l-k}\right)\right. \\
&\quad \left. + \sum_{k=1}^{l-2}\left(\sum_{i=1}^{l-1-k}(l + i - k)2^{l+i-k-1}\right) + \sum_{i=1}^{l-1}\left(\sum_{j=1}^{i} 2j \times 2^{j-1}\right)2^{i-1}\right] \\
&= 8l \times 2^l - 36 \times 2^{2l} + 38 \times 2^l + 16l \times 2^{2l} - 2.
\end{aligned}
$$

Theorem 3.2.7 *Let $T_l, l \geq 2$ be the complete binary tree network of level l. Then the Gutman index*

$$Gut(T_l) = 8l \times 2^l - 40 \times 2^{2l} + 46 \times 2^l + 16l \times 2^{2l} - 6.$$

The proof runs analogous to that of Theorem 3.2.6.

Remark 3.2.8 The results obtained from TopoChemie-2020 are shown in Table 3 for comparison with the results obtained from Theorems 3.2.1–3.2.7.

4 Conclusion

The various recursive structures that we have considered in the present study are not only applicable to mitigation strategies for control of COVID-19 but also in a number of other applications such as neural networks in characterization of toxicity profiles [24], population dynamics, social or technological networks, genome networks, proteomics

networks, and metabolomics networks. Hence the tools developed here could have wide ranging applications in a number of disciplines. The various topological indices derived here serve to provide label-independent quantification measures for the networks, especially in measuring perturbations that would be caused by the addition of edges or vertices which would then model for example, the effect of the introduction of an infected individual in a pool of uninfected individuals. In the present study we have considered various topological indices of such recursive tree structures and phylogenetic trees of interest in biochemical and epidemiological applications with the potentials to develop further variants in the future that would measure the causal effects of perturbations into a network through an infected individual. In addition to purely biological applications, recursive tree networks such as binary trees and higher order trees can provide topological insights into molecular dendrimers and their relativistic extensions can be especially of future significance in structure–activity relations pertinent to metal–organic frameworks for which relativistic effects could become important [25–29]. Recently we have applied such networks and their topological indices to pandemic networks relevant to COVID-19 [30].

Compliance with ethical standards

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

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