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Extended study of biological networks using graph theory

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Abstract

We represent biological networks by a function that maps the structure of a network to a number called topological index. Topological indices have been studied for biological networks in which a person transmits a virus to two other people, and a person having the virus is in contact with exactly one other person who got the virus from someone else. We extend research in this area by studying biological networks in which a person transmits a virus to n other people, where $n \geq 2$, and a person having the virus is in contact with p other people ($0 \leq p \leq n-2$) who got the virus from some other person.

Keywords: *Topological index, virus, biological network.*

Mathematics Subject Classification: *05C09, 05C90.*

1. Introduction

Topological indices measure physical, chemical and biological properties. We represent biological networks by a function that maps the structure of a network to a number called topological index.

Biological networks $HT(h)$ and ST_h^1 were studied by Imran et al. [7] and Gao et al. [4]; see Figures 1 and 2. They assume that a virus or bacteria is transmitted from one person to two other people, and a person having the virus is in contact with exactly one other person who got the virus from someone else. We extend research in this area by studying biological networks in which a virus or bacteria is transmitted from one person to n other people, where $n \geq 2$, and a person having the virus is in contact with p other people ($0 \leq p \leq n-2$) who got the virus from someone else.

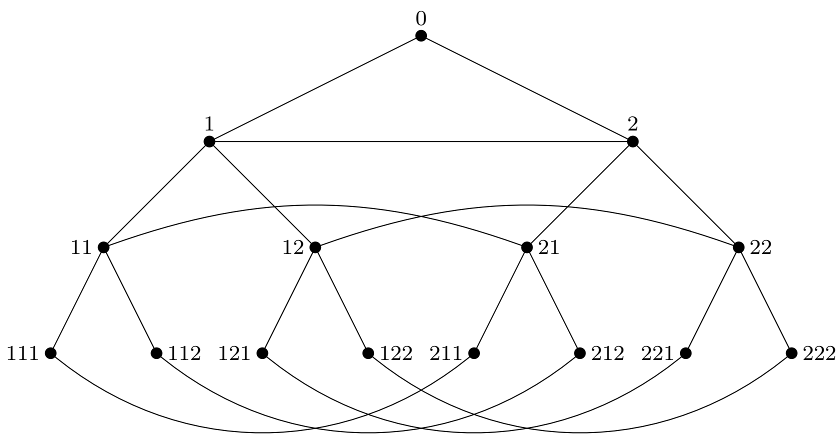

Figure 1: Network $HT(h)$ for $h = 3$.

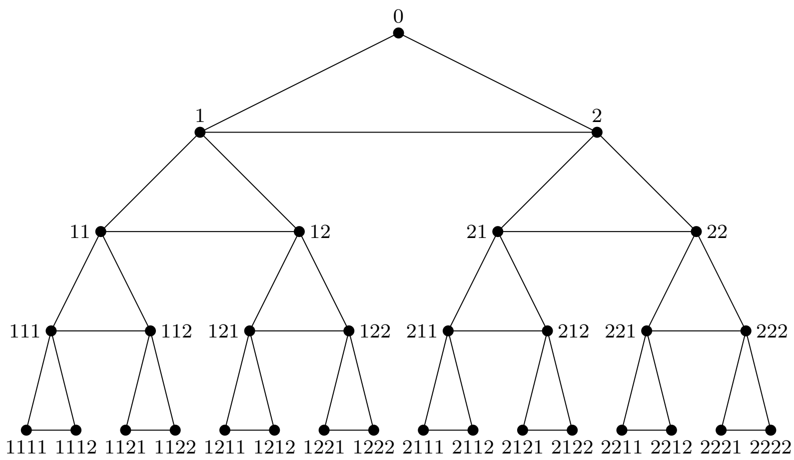

Figure 2: Network ST_h^1 for $h = 3$.

Let $V(N)$ be the vertex set and $E(N)$ be the edge set of a network N. The number of edges in a shortest path between two vertices is called the distance between those two vertices. The distance between u and a vertex farthest from u is called the eccentricity $ecc_N(u)$ of a vertex u in N.

We define complete n-ary trees $T_{n,h}$ of given height $h \geq 1$. Those tress are used to define our extended biological networks. The vertices of $T_{n,h}$ are partitioned into $h+1$ sets $S_0, S_1, \ldots, S_h$. For $i = 1, 2, \ldots, h$,

$$\mathrm{S}_i = \{(v_1, v_2, \ldots, v_i) \mid 1 \leq v_j \leq n;\ j = 1, 2, \ldots, i\}.$$

A vertex $(v_1, v_2, \ldots, v_i)$ is sometimes denoted by $v_1 v_2 \ldots v_i$. The root 0 is the only vertex of S_0 and it is joined to the n vertices of S_1. For $i = 1, 2, \ldots, h-1$, Each vertex $(v_1, v_2, \ldots, v_i)$ of S_i is joined to

$$(\mathrm{v}_1, v_2, \ldots, v_i, 1), (v_1, v_2, \ldots, v_i, 2), \ldots, (v_1, v_2, \ldots, v_i, n)$$

of S_{i+1}.

For $p = 0, 1, 2, \ldots, n-2$, the set $T_{n,h}^p$ includes the networks created from $T_{n,h}$ by joining every vertex v in S_i (where $i = 2, 3, \ldots, h$) to any p vertices in S_i which have the first entry equal to the first entry of v, and by joining every vertex in S_1 to any p vertices in S_1. Note that this construction is possible only if at least one of the integers p and n is even. So, the set $T_{n,h}^p$ is empty if both p and n are odd. One network of $T_{n,h}^p$ for $p = 2$, $n = 5$

and $h = 2$ is given in Figure 3.

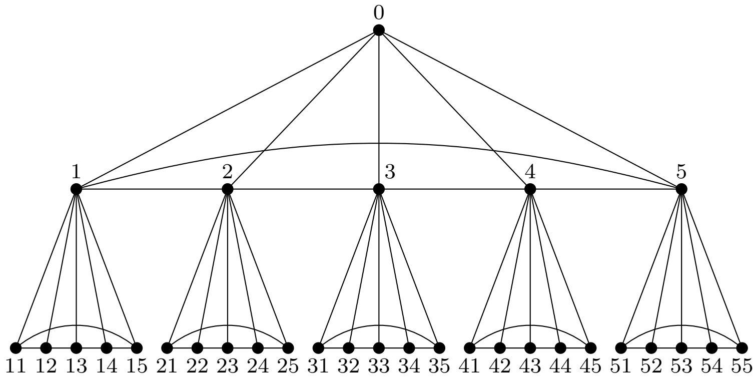

Figure 3: Network in $T^p_{n,h}$ for $p = 2$, $n = 5$ and $h = 2$.

For any network $N \in T^p_{n,h}$, a vertex in $V(N) \setminus (S_0 \cup S_1)$ having the first entry j is not joined to a vertex having the first entry l, where $j \neq l$. Thus, for $i = 1, 2, \ldots, h$, the eccentricity of $(v_1, v_2, \ldots, v_i) \in S_i$ is $h + i$. Any vertex $(u_1, u_2, \ldots, u_h) \in S_h$, where (u_1) is not adjacent to (v_1) is a farthest vertex from $(v_1, v_2, \ldots, v_i)$.

The path

$$(v_1, v_2, \ldots, v_i), (v_1, v_2, \ldots, v_{i-1}), \ldots, (v_1), 0, (u_1), (u_1, u_2), \ldots, (u_1, u_2, \ldots, u_h)$$

is the shortest path connecting $(v_1, v_2, \ldots, v_i)$ and $(u_1, u_2, \ldots, u_h)$. Note that the eccentricity of 0 is h in $T^p_{n,h}$,

The first Zagreb eccentricity index of a network N,

$$\xi_1(N) = \sum_{u \in V(N)} (ecc_N(u))^2$$

and the second Zagreb eccentricity index

$$\xi_2(N) = \sum_{uv \in E(N)} ecc_N(u) ecc_N(v)$$

were defined in [11]. The ξ_1' index

$$\xi_1'(N) = \sum_{uv \in E(N)} (ecc_N(u) + ecc_N(v))$$

was defined in [5]. The modified Zagreb eccentricity index is the name which will be used for the ξ_1' index.

For $a \in \mathbf{R}$, we define the general eccentricity index

$$EI_a(N) = \sum_{u \in V(N)} (ecc_N(u))^a.$$

The total eccentricity index

$$EI_1(N) = \sum_{u \in V(N)} ecc_N(u)$$

is obtained when using $a = 1$ and the first Zagreb eccentricity index $EI_2 = \xi_1$ is obtained when using $a = 2$.

Zagreb eccentricity indices have been investigated due to their wide applications. Eccentricity based indices of honeycomb networks were studied in [6], nanostar dendrimers in [3] and oxid networks in [8], For related works, see [1], [2], [9] and [10].

2. Results

Let $n \geq 2$ and $h \geq 1$ be positive integers. In our main results we often use $\sum_{i=c}^{h} n^i$, $\sum_{i=c}^{h} in^i$ and $\sum_{i=c}^{h} i^2 n^i$ for $c = 0$ and $c = 1$, therefore we present the values of these sums first. We have

$$\sum_{i=0}^{h} n^i = \frac{n^{h+1} - 1}{n - 1} \quad \text{and} \quad \sum_{i=1}^{h} n^i = \frac{n(n^h - 1)}{n - 1}.$$

Then

$$(1-n)\sum_{i=0}^{h} in^i = n + n^2 + n^3 + \ldots + n^h - hn^{h+1} = \frac{n(1-n^h)}{1-n} - hn^{h+1}$$

and

$$\sum_{i=0}^{h} in^i = \frac{n(1-n^h)}{(1-n)^2} + \frac{hn^{h+1}}{n-1} = \frac{hn^{h+2} - (h+1)n^{h+1} + n}{(n-1)^2}.$$

Since $(n-1)^2 \sum_{i=0}^{h} i^2 n^i$

$$\begin{aligned}
&= n + 2n^2 + 2n^3 + 2n^4 + \ldots + 2n^h - (h^2 + 2h - 1)n^{h+1} + h^2 n^{h+2} \\
&= n + 2n^2(1 + n + n^2 + \ldots + n^{h-2}) - (h^2 + 2h - 1)n^{h+1} + h^2 n^{h+2} \\
&= \frac{2n^2(n^{h-1} - 1)}{n-1} + n - (h^2 + 2h - 1)n^{h+1} + h^2 n^{h+2},
\end{aligned}$$

we obtain

$$\begin{aligned}\sum_{i=0}^{h} i^2 n^i &= \frac{2n^{h+1}-2n^2}{(n-1)^3} + \frac{h^2 n^{h+2} - (h^2+2h-1)n^{h+1} + n}{(n-1)^2} \\ &= \frac{h^2 n^{h+3} - (2h^2+2h-1)n^{h+2} + (h+1)^2 n^{h+1} - n^2 - n}{(n-1)^3}.\end{aligned}$$

Note that $\sum_{i=0}^{h} in^i = \sum_{i=1}^{h} in^i$ and $\sum_{i=0}^{h} i^2 n^i = \sum_{i=1}^{h} i^2 n^i$.

All the theorems presented in this paper hold for $h \geq 1$ and $0 \leq p \leq n-2$, where at least one of the integers p and n is even. For $a \in \mathbf{R}$, we study the general eccentricity index EI_a of networks in $T^p_{n,h}$.

Theorem 1. *Let N be any network in $T^p_{n,h}$. Then*

$$EI_a(N) = \sum_{i=0}^{h} n^i (h+i)^a.$$

Proof. In N, the number of vertices of S_i is n^i, where $i = 0, 1, 2, \ldots, h$. The eccentricity of each vertex in S_i is $h+i$. Therefore

$$\begin{aligned}EI_a(N) &= \sum_{u \in S_0} h^a + \sum_{u \in S_1} (h+1)^a + \sum_{u \in S_2} (h+2)^a + \ldots + \sum_{u \in S_h} (2h)^a \\ &= n^0 h^a + n^1 (h+1)^a + n^2 (h+2)^a + \ldots + n^h (2h)^a \\ &= \sum_{i=0}^{h} n^i (h+i)^a\end{aligned}$$

□

The total eccentricity index EI_1 of any biological network from the set $T^p_{n,h}$ is studied in Theorem 2.

Theorem 2. *Let N be any network in $T^p_{n,h}$. Then*

$$EI_1(N) = \frac{2hn^{h+2} - (2h+1)n^{h+1} - hn + n + h}{(n-1)^2}.$$

Proof. From Theorem 1, we obtain

$$EI_1(N) = \sum_{i=0}^{h} n^i (h+i).$$

Thus

$$\begin{aligned} EI_1(N) &= h\sum_{i=0}^{h} n^i + \sum_{i=0}^{h} in^i \\ &= \frac{hn^{h+1}-h}{n-1} + \frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2} \\ &= \frac{2hn^{h+2}-(2h+1)n^{h+1}-hn+n+h}{(n-1)^2}. \end{aligned}$$

□

The first Zagreb eccentricity index ξ_1 $(= EI_2)$ is investigated in Theorem 3.

Theorem 3. *Let N be any network in $T^p_{n,h}$. Then*

$$\begin{aligned} \xi_1(N) &= \frac{4h^2n^{h+3}-(6h^2+6h-1)n^{h+2}+(2h+1)^2n^{h+1}-(h-1)^2n^2}{(n-1)^3} \\ &\quad + \frac{(2h^2-2h-1)n-h^2}{(n-1)^3}. \end{aligned}$$

Proof. From Theorem 1, we obtain

$$EI_2(N) = \xi_1(N) = \sum_{i=0}^{h} n^i (h+i)^2.$$

Thus

$$\begin{aligned} \xi_1(N) &= \sum_{i=0}^{h} n^i (h^2+2hi+i^2) \\ &= h^2\sum_{i=0}^{h} n^i + 2h\sum_{i=0}^{h} in^i + \sum_{i=0}^{h} i^2 n^i \end{aligned}$$

$$= h^2\left(\frac{n^{h+1}-1}{n-1}\right)+2h\left(\frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2}\right)$$
$$+\frac{h^2n^{h+3}-(2h^2+2h-1)n^{h+2}+(h+1)^2n^{h+1}-n^2-n}{(n-1)^3}$$
$$= \frac{4h^2n^{h+3}-(6h^2+6h-1)n^{h+2}+(2h+1)^2n^{h+1}-(h-1)^2n^2}{(n-1)^3}$$
$$+\frac{(2h^2-2h-1)n-h^2}{(n-1)^3}.$$

□

Let us introduce the general invariant

$$I(G)=\sum_{uv\in E(G)} f(ecc_N(u),ecc_N(v)),$$

with $f(ecc_N(u),ecc_N(v))$ being a function of $ecc_N(u)$ and $ecc_N(v)$ where $f(ecc_N(u),ecc_N(v))=f(ecc_N(v),ecc_N(u))$.

The second Zagreb eccentricity index is obtained if $f(ecc_N(u),ecc_N(v))=ecc_N(u)ecc_N(v)$. The modified Zagreb eccentricity index is obtained if $f(ecc_N(u),ecc_N(v))=ecc_N(u)+ecc_N(v)$.

Theorem 4. *Let N be any network in $T^p_{n,h}$. Then*

$$I(N)=\sum_{i=1}^{h}\left[n^if(h+i-1,h+i)+\frac{pn^i}{2}f(h+i,h+i)\right].$$

Proof. The number of edges in N is

$$\left(n+n^2+\ldots+n^h\right)+\left(\frac{pn}{2}+\frac{pn^2}{2}+\ldots+\frac{pn^h}{2}\right).$$

Let

$$E_{j,l}=\{uv\in E(N)\mid u\in S_j,\ v\in S_l\}.$$

We have

$$E(N)=(E_{1,1}\cup E_{2,2}\cup\ldots\cup E_{h,h})\cup(E_{0,1}\cup E_{1,2}\cup\ldots\cup E_{h-1,h}).$$

We get

$$|E_{0,1}| = n^1,\ |E_{1,2}| = n^2, \ldots,\ |E_{h-1,h}| = n^h$$

and

$$|E_{1,1}| = \frac{pn}{2},\ |E_{2,2}| = \frac{pn^2}{2}, \ldots,\ |E_{h,h}| = \frac{pn^h}{2}.$$

Each vertex in S_i is of eccentricity $h+i$, where $i = 0, 1, 2, \ldots, h$, therefore

$$\begin{aligned}
I(N) &= \sum_{uv \in E(N)} f(ecc_N(u), ecc_N(v)) \\
&= \sum_{uv \in E_{0,1}} f(h, h+1) + \sum_{uv \in E_{1,2}} f(h+1, h+2) + \ldots \\
&\quad + \sum_{uv \in E_{h-1,h}} f(2h-1, 2h) \\
&\quad + \sum_{uv \in E_{1,1}} f(h+1, h+1) + \sum_{uv \in E_{2,2}} f(h+2, h+2) + \ldots \\
&\quad + \sum_{uv \in E_{h,h}} f(2h, 2h) \\
&= n \cdot f(h, h+1) + n^2 f(h+1, h+2) + \ldots + n^h f(2h-1, 2h) \\
&\quad + \frac{pn}{2} f(h+1, h+1) + \frac{pn^2}{2} f(h+2, h+2) + \ldots + \frac{pn^h}{2} f(2h, 2h) \\
&= \sum_{i=1}^{h} n^i f(h+i-1, h+i) + \sum_{i=1}^{h} \frac{pn^i}{2} f(h+i, h+i).
\end{aligned}$$

□

We use Theorem 4 to study the ξ_1' and ξ_2 indices of biological networks.

Theorem 5. *Let N be any network in $T^p_{n,h}$. Then the modified Zagreb eccentricity index*

$$\begin{aligned}
\xi_1'(N) &= \frac{(2ph+4h-1)n^{h+2} - (2ph+4h+p+1)n^{h+1} - (ph+2h-1)n^2}{(n-1)^2} \\
&\quad + \frac{(ph+2h+p+1)n}{(n-1)^2}
\end{aligned}$$

and the second Zagreb eccentricity index

$$\xi_2(N) = h\left(\frac{ph}{2}+h-1\right)\frac{n^{h+1}-n}{n-1}+(ph+2h-1)\frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2} + \left(\frac{p}{2}+1\right)\left[\frac{h^2n^{h+3}-(2h^2+2h-1)n^{h+2}+(h+1)^2n^{h+1}-n^2-n}{(n-1)^3}\right].$$

Proof. We have $f(ecc_N(u), ecc_N(v)) = ecc_N(u) + ecc_N(v)$ in the case of ξ'_1 index. Thus $f(h+i-1, h+i) = 2h+2i-1$ and $f(h+i, h+i) = 2h+2i$. From Theorem 4, we get

$$\begin{aligned}
\xi'_1(N) &= \sum_{i=1}^{h}\left[n^i(2h+2i-1)+\frac{pn^i}{2}(2h+2i)\right] \\
&= (ph+2h-1)\sum_{i=1}^{h} n^i + (p+2)\sum_{i=1}^{h} in^i \\
&= (ph+2h-1)\frac{n(n^h-1)}{n-1}+(p+2)\frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2} \\
&= \frac{(2ph+4h-1)n^{h+2}-(2ph+4h+p+1)n^{h+1}-(ph+2h-1)n^2}{(n-1)^2} \\
&\quad +\frac{(ph+2h+p+1)n}{(n-1)^2}.
\end{aligned}$$

We have $f(ecc_N(u), ecc_N(v)) = ecc_N(u)ecc_N(v)$ in the case of ξ_2 index. Thus $f(h+i-1, h+i) = (h+i-1)(h+i) = h^2-h+2hi-i+i^2$ and $f(h+i, h+i) = (h+i)(h+i) = h^2+2hi+i^2$. From Theorem 4, we get

$$\begin{aligned}
\xi_2(N) &= \sum_{i=1}^{h}\left[n^i(h^2-h+2hi-i+i^2)+\frac{pn^i}{2}(h^2+2hi+i^2)\right] \\
&= h\left(\frac{ph}{2}+h-1\right)\sum_{i=1}^{h} n^i + (ph+2h-1)\sum_{i=1}^{h} in^i + \left(\frac{p}{2}+1\right)\sum_{i=1}^{h} i^2n^i \\
&= h\left(\frac{ph}{2}+h-1\right)\frac{n^{h+1}-n}{n-1}+(ph+2h-1)\frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2} \\
&\quad +\left(\frac{p}{2}+1\right)\left[\frac{h^2n^{h+3}-(2h^2+2h-1)n^{h+2}+(h+1)^2n^{h+1}-n^2-n}{(n-1)^3}\right].
\end{aligned}$$

□

In Corollary 1, we consider the situation when a person having a virus is in contact with one other person who got the virus from someone else. So $p = 1$. See Figure 4 for the case in which a person transmits the virus to 4 other people, so $n = 4$.

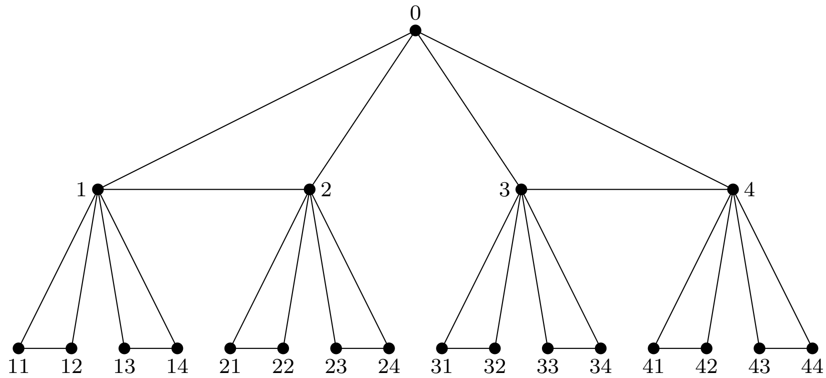

Figure 4: One of the network in $T^p_{n,h}$ for $p = 1$, $n = 4$ and $h = 2$.

Corollary 1. *Let N be any network in $T^1_{n,h}$, where $n \geq 4$ is even and $h \geq 1$. Then the modified Zagreb eccentricity index*

$$\xi_1'(N) = \frac{(6h-1)n^{h+2} - (6h+2)n^{h+1} - (3h-1)n^2 + (3h+2)n}{(n-1)^2}$$

and the second Zagreb eccentricity index

$$\xi_2(N) = \frac{4h(3h-1)n^{h+3} - (24h^2+4h-5)n^{h+2} + (2h+1)(6h+1)n^{h+1}}{2(n-1)^3} + \frac{h(2-3h)n^3 + (6h^2+2h-5)n^2 - (3h^2+4h+1)n}{2(n-1)^3}.$$

Proof. We use $p = 1$ in Theorem 5 to obtain

$$\xi_1'(N) = \frac{(6h-1)n^{h+2} - (6h+2)n^{h+1} - (3h-1)n^2 + (3h+2)n}{(n-1)^2}$$

and

$$\begin{aligned}\xi_2(N) &= h\left(\frac{3h-2}{2}\right)\frac{n^{h+1}-n}{n-1}+(3h-1)\frac{hn^{h+2}-(h+1)n^{h+1}+n}{(n-1)^2}\\&+\frac{3}{2}\left[\frac{h^2n^{h+3}-(2h^2+2h-1)n^{h+2}+(h+1)^2n^{h+1}-n^2-n}{(n-1)^3}\right]\\&= \frac{4h(3h-1)n^{h+3}-(24h^2+4h-5)n^{h+2}+(2h+1)(6h+1)n^{h+1}}{2(n-1)^3}\\&+\frac{h(2-3h)n^3+(6h^2+2h-5)n^2-(3h^2+4h+1)n}{2(n-1)^3}.\end{aligned}$$

□

It is easy to check that for example for $p = 1$ and $h = 2$, we get $\xi_1'(N) = 11n^2 + 8n$ and $\xi_2(N) = 20n^2 + \frac{21}{2}n$.

In Corollary 2, we consider the case when a person having the virus is not in contact with people who got the virus from someone else. So $p = 0$. For each $n \geq 2$ and $h \geq 1$, the only tree in the set $T^0_{n,h}$ is the complete n-ary tree of height h; see Figure 5.

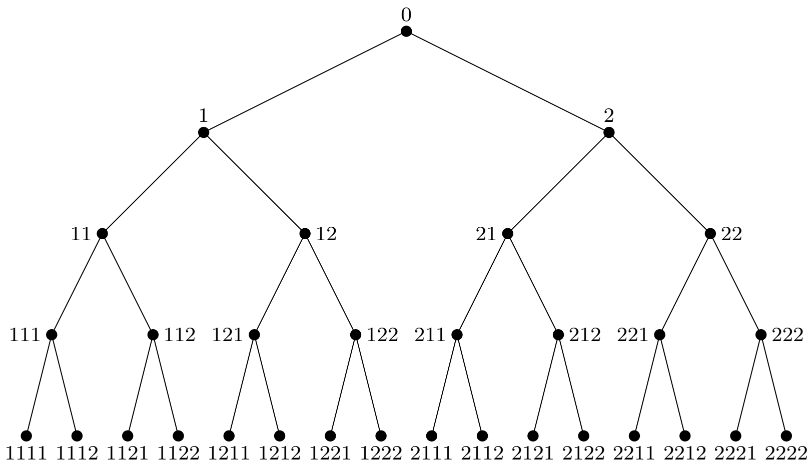

Figure 5: Complete n-ary tree $T_{n,h}$ for $n = 2$ and $h = 4$.

Corollary 2. *For the complete n-ary tree $T_{n,h}$ of height h, where $n \geq 2$ and $h \geq 1$, we get*

$$\xi_1'(T_{n,h}) = \frac{(4h-1)n^{h+2}-(4h+1)n^{h+1}-(2h-1)n^2+(2h+1)n}{(n-1)^2}$$

and

$$\xi_2(T_{n,h}) = \frac{2h(2h-1)n^{h+3} - (8h^2-2)n^{h+2} + 2h(2h+1)n^{h+1}}{(n-1)^3} - \frac{h(h-1)n^3 + 2(h^2-1)n^2 - h(h+1)n}{(n-1)^3}.$$

Proof. We use $p = 0$ in Theorem 5 to obtain the ξ_1' index of $T_{n,h} \in T_{n,h}^0$,

$$\xi_1'(T_{n,h}) = \frac{(4h-1)n^{h+2} - (4h+1)n^{h+1} - (2h-1)n^2 + (2h+1)n}{(n-1)^2}$$

and

$$\begin{aligned}\xi_2(T_{n,h}) &= h(h-1)\frac{n^{h+1}-n}{n-1} + (2h-1)\frac{hn^{h+2} - (h+1)n^{h+1} + n}{(n-1)^2} \\ &\quad + \frac{h^2n^{h+3} - (2h^2+2h-1)n^{h+2} + (h+1)^2n^{h+1} - n^2 - n}{(n-1)^3} \\ &= \frac{2h(2h-1)n^{h+3} - (8h^2-2)n^{h+2} + 2h(2h+1)n^{h+1}}{(n-1)^3} \\ &\quad - \frac{h(h-1)n^3 + 2(h^2-1)n^2 - h(h+1)n}{(n-1)^3}.\end{aligned}$$

□

It is easy to check that for example for $h = 2$, we get $\xi_1'(T_{n,h}) = 7n^2 + 5n$ and $\xi_2(T_{n,h}) = 12n^2 + 6n$.

3. Conclusion

Gao et al. [4] and Imran et al. [7] investigated biological networks assuming that a virus is transmitted from one person to two other people, and a person having the virus is in contact with exactly one other person who got the virus from someone else. We extended research in this area by studying biological networks in which a person transmits a virus to n other people, where $n \geq 2$, and a person having the virus is in contact with p other people ($0 \leq p \leq n-2$) who got the virus from someone else. We obtain eccentricity based indices of these biological networks.

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