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ON TOPOLOGICAL CHARACTERIZATION OF HIERARCHICAL HYPERCUBE INTERCONNECTION NETWORKS USING M-POLYNOMIALS

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Abstract: The application of the M-polynomial to chemical networks, particularly to chemical compounds, is a relatively recent development in chemical graph theory. Despite its novelty, this approach has proven to be a powerful and effective tool for deriving degree-based topological indices. These indices play a crucial role in modeling and predicting various physicochemical properties as well as biological activities of chemical substances and nanostructured systems. The M-polynomial offers a unified and systematic framework by establishing mathematical relationships between molecular structure and chemical behavior. In this work, we focus on computing the general

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form of M-polynomials for Hierarchical Hypercube Networks (HHNs). The selected HHNs exhibit a high degree of structural symmetry, which significantly simplifies the analytical computations and enables the exact determination of the corresponding M-polynomials. By exploiting these symmetries, we derive closed-form expressions that describe the underlying degree distributions of the considered nanostructures. Furthermore, several important degree-based topological indices are obtained from the derived M-polynomials. These indices provide valuable insights into the structural complexity and potential chemical dynamics of the studied Hierarchical Hypercube Networks. Finally, the M-polynomials are presented graphically to highlight and visualize the structural characteristics of the HHNs.

Keywords: Hierarchical Hypercube Networks (HHNs); M-polynomials; Topological descriptors; Entropies.

2020 AMS Subject Classification: 05C09, 05C92.

1. INTRODUCTION

In chemistry, a molecular graph is a mathematical abstraction applied in chemical graph theory to determine the structure of a chemical compound. Informally, a molecular graph is a simple graph, that is, it does not have loops (edges of both ends of the edge point to the same vertex) nor does it have multiple edges (two edges between similar pairs of vertices). This representation has atoms of a molecule being represented as the vertices, and chemical bonding between atoms represented as edges.

Topological indices refer to invariants of molecular graphs which are numbers. They are calculated based on the graph structure of a chemical compound and they are invariant with graph isomorphisms. Topological indices are useful in quantitative structure-property relationships (QSPR), quantitative structure-activity relationships (QSAR), in which molecular structure is associated with physical, chemical, or biological properties due to this invariance.

Another family of topological indices is of great particular interest and is obtained with the degrees of the vertices in the molecular graph. These indices are referred to as degree-based topological indices. These indices relate critical structural data of a molecule since they encode the links of atoms with varying valencies. The most famous ones are the Zagreb indices, hyper-Zagreb indices and numerous of their variants. degree-based topological indices are highly predictive and computationally simple and it has been shown that they have wide application and research in chemical graph theory [1-7].

Intimately connected with degree based topological indices is the M-polynomial concept. M-polygonal representation of a molecular graph represents shortly the shape of the distribution of locations given the edge degrees of their end nodes. The key benefit of it is that it can be used to obtain many degree-based topological indices as direct extensions of the M-polynomial, which is achieved by using appropriate differential or algebraic operators. As such, the M-polynomial gives a unified expression of closed-form expressions to a large number of degree-based topological indices [8-13].

Over the last several years, a body of literature has been dedicated to computing the M-polynomial and similar topological data sets, of a variety of chemical graph classes, especially the dendrimer and nanostructure classes of the chemical graph. As an illustration, the authors of [14] examined two families of nanostar dendrimers, which were infinitely generated (that is, denoted by (NS_1[n]) and (NS_2[n]) and determined their Zagreb indices and Zagreb polynomials. Some Zagreb polynomials have been calculated in [15] for a special form of dendrimer nanostar (D_3[n]), and a larger investigation of the Zagreb indices and Zagreb polynomials of the same nanostar dendrimers was performed in [16].

Other contributions involve the calculation of some fifth multiplicative Zagreb indices of dendrimers as was reported in [17]. The authors in [18] investigated some reverse degrees-based descriptors, such as the first and the second reverse Zagreb indices, reverse hyper-Zagreb indices, as well as their respective polynomials, of porphyrin, propyl ether imine, zinc porphyrin, and poly(ethylene amido amine) dendrimers. Also, M-polynomial and other topological indices of a benzene ring embedded in P-type surface network were acquired in [19]. In [12], the M-polynomial, metric dimension and topological indices of polyhex nanotubes were investigated with reference to degrees, the application of topological indices, coherence and robustness analysis for a family of unbalanced networks is discussed and many others computer-based problems are discussed in [20-25].

In this paper, the Hierarchical Hypercube Networks (HHNs) are considered for developing the topological indices and entropies on it. The rest of the paper arranges as: In section 2, the mathematical form of topological indices and entropies are discussed. In section 3, the Hierarchical Hypercube Networks (HHNs) and their partition function with respect to degrees of the end points of the edges are considered. In section 4 and 5, the various topological indices for HHN_1, HHN_2 are computed respectively, further their numerical and graphical comparisons are developed in these sections. In section 6, two kind of entropies are investigated for for HHN_1, HHN_2.

2. TOPOLOGICAL INDICES, M-POLYNOMIALS AND ENTROPIES

In this section, we will discuss about some well-known topological indices, then discuss their relations with M-polynomials. Further, entropies which are based on the degrees of the end points of edges are considered. The well-known topological indices with their mathematical expression, and M-polynomials are developed in [26-40]. The two well-known entropies are developed in [41, 42].

Table 1: Some well-known topological indices with their mathematical expression.

TI	Mathematical Expression
$M_1(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} (\mathfrak{D}(\mathfrak{s}_1)+\mathfrak{D}(\mathfrak{s}_2))$
$M_2(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2)$
${}^{m}M_2(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \frac{1}{\mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2)}$
$R_\alpha(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} (\mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2))^\alpha$
$RR_\alpha(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \frac{1}{(\mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2))^\alpha}$
$SSD_3(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2)(\mathfrak{D}(\mathfrak{s}_1)+\mathfrak{D}(\mathfrak{s}_2))$
$SSD_5(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \left(\frac{\mathfrak{D}(\mathfrak{s}_1)}{\mathfrak{D}(\mathfrak{s}_2)}+\frac{\mathfrak{D}(\mathfrak{s}_2)}{\mathfrak{D}(\mathfrak{s}_1)}\right)$
$I(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \left(\frac{\mathfrak{D}(\mathfrak{s}_1)\mathfrak{D}(\mathfrak{s}_2)}{\mathfrak{D}(\mathfrak{s}_1)+\mathfrak{D}(\mathfrak{s}_2)}\right)$
$H(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} \left(\frac{2}{\mathfrak{D}(\mathfrak{s}_1)+\mathfrak{D}(\mathfrak{s}_2)}\right)$
$F(G)$	$\sum_{\mathfrak{s}_1\mathfrak{s}_2\in E(G)} (\mathfrak{D}(\mathfrak{s}_1)^2+\mathfrak{D}(\mathfrak{s}_2)^2)$

The M-polynomial of a graph is defined as [9]

$$M(G;\, \mathfrak{s}_1,\, \mathfrak{s}_2) = \sum_{\alpha \le \beta} \rho(\alpha, \beta)\, {\mathfrak{s}_1}^{\alpha}\, {\mathfrak{s}_2}^{\beta}$$

In Table 2 the relationship with topological indices and M-polynomial, and In Table 3 some well-known entropies are given.

Table 2: Relationship with topological indices and M-polynomial.

TI	Mathematical Expression
$M_1(G)$	$\left[\left(D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$M_2(G)$	$\left[\left(D_{\mathfrak{s}_1} D_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
${}^{m}M_2(G)$	$\left[\left(S_{\mathfrak{s}_1} S_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$R_{\alpha}(G)$	$\left[\left(D^{\alpha}_{\mathfrak{s}_1} D^{\alpha}_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$RR_{\alpha}(G)$	$\left[\left(S^{\alpha}_{\mathfrak{s}_1} S^{\alpha}_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$SSD_3(G)$	$\left[D_{\mathfrak{s}_1} D_{\mathfrak{s}_2}\left((D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2})\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$SSD_5(G)$	$\left[\left(S_{\mathfrak{s}_1} D_{\mathfrak{s}_1} + S_{\mathfrak{s}_2} D_{\mathfrak{s}_2}\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$
$I(G)$	$\left[2S_{\mathfrak{s}_1} J\left(\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1)=(1)}$
$H(G)$	$\left[S_{\mathfrak{s}_1} J_{\ \mathfrak{s}_1} D_{\mathfrak{s}_2}\left(\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1)=(1)}$
$F(G)$	$\left[({D_{\mathfrak{s}_1}}^2 + {D_{\mathfrak{s}_2}}^2)\left(\left(M(G, \quad \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right] \mid_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$

Where

$$D_{\mathfrak{s}_1} = \mathfrak{s}_1\left(\frac{\partial(M(G, \mathfrak{s}_1, \mathfrak{s}_2))}{\partial\, \mathfrak{s}_1}\right), \qquad D_{\mathfrak{s}_2} = \mathfrak{s}_2\left(\frac{\partial(M(G, \mathfrak{s}_1, \mathfrak{s}_2)}{\partial\, \mathfrak{s}_2}\right), \quad S_{\mathfrak{s}_1} = \int_0^{\mathfrak{s}_1} M(G, t, \mathfrak{s}_2)/t\ \mathfrak{D}t,$$

$$S_{\mathfrak{s}_2} = \int_0^{\mathfrak{s}_2} M(G, \mathfrak{s}_1, t)/t\, \mathfrak{D}t, \quad J = M(G, \mathfrak{s}_1, \mathfrak{s}_2), \qquad Q_a = \mathscr{b}^{a} M(G, \mathfrak{s}_1, \mathfrak{s}_2), a \neq 0$$

Table 3: Some well-known entropies with mathematical expressions.

Entropies	Mathematical Expression
$ENT_{ReZE_1(G)}$	$\log(ReZG_1) - \frac{1}{ReZG_1}\log\left\{\prod_{b_i, f_j \in E(G_1)} \left[\frac{\zeta_{b_i} + \zeta_{f_j}}{\zeta_{b_i}\zeta_{f_j}}\right]^{\left[\frac{\zeta_{b_i}+\zeta_{f_j}}{\zeta_{b_i}\zeta_{f_j}}\right]}\right\}$
$ENT_{ReZE_2(G)}$	$\log(ReZG_2) - \frac{1}{ReZG_2}\log\left\{\prod_{b_i, f_j \in E(G_2)} \left[\frac{\zeta_{b_i}\zeta_{f_j}}{\zeta_{b_i}+\zeta_{f_j}}\right]^{\left[\frac{\zeta_{b_i}\zeta_{f_j}}{\zeta_{b_i}+\zeta_{f_j}}\right]}\right\}$
$ENT_{ReZE_3(G)}$	$\log(ReZG_3) - \frac{1}{ReZG_3}\log\left\{\prod_{b_i, f_j \in E(G_3)} \left[(\zeta_{b_i}\zeta_{f_j})(\zeta_{b_i} + \zeta_{f_j})\right]^{\left[(\zeta_{b_i}\zeta_{f_j})(\zeta_{b_i}+\zeta_{f_j})\right]}\right\}$

Where

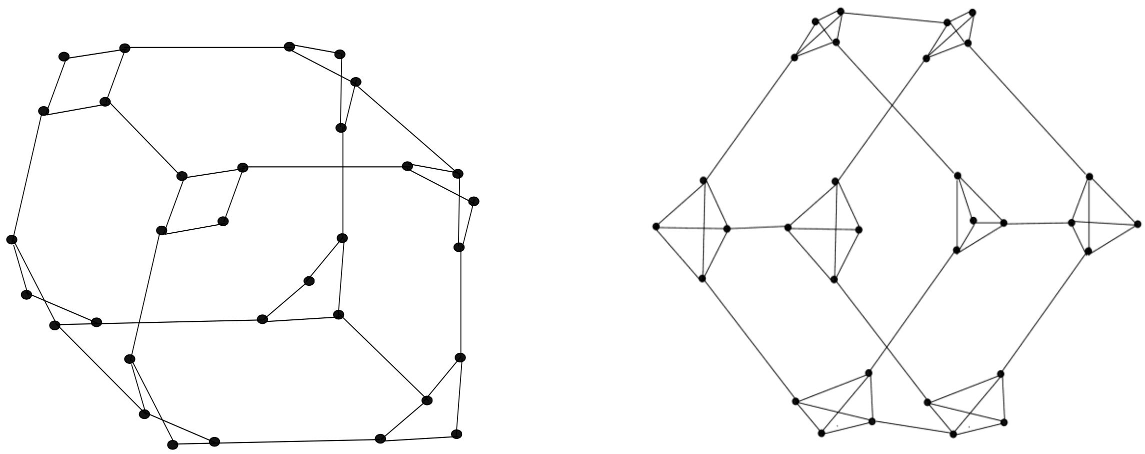
$$ReZG_1(G) = \sum_{b_i, f_j \in E(G)} \left\{\frac{\zeta_{b_i}+\zeta_{f_j}}{\zeta_{b_i}\zeta_{f_j}}\right\}$$

$$ReZG_2(G) = \sum_{b_i, f_j \in E(G)} \left\{\frac{\zeta_{b_i}\zeta_{f_j}}{\zeta_{b_i}+\zeta_{f_j}}\right\}$$

$$ReZG_3(G) = \sum_{b_i, f_j \in E(G)} \left\{(\zeta_{b_i}\zeta_{f_j})(\zeta_{b_i} + \zeta_{f_j})\right\}$$

3. HIERARCHICAL HYPERCUBE NETWORKS

Hierarchical Hypercube Networks (HHNs) are an important class of interconnection networks studied in graph theory and parallel/distributed computing. They are designed to overcome some limitations of classical hypercube graphs (such as scalability and wiring complexity) while preserving desirable properties like symmetry and low diameter. In Figures (a) and (b) depict the two hierarchical hypercube networks, HHN_1 and HHN_2, respectively. In HHN_1, there are 16*n*+16 vertices and 24*n*+20 edges in total, respectively. The total numbers of vertices and edges in HHN_2 are 16*n* + 16 and 32*n* + 28, respectively, as shown in Figure (b).



(a) $(HHN_1)_{1\times1}$ (b) $(HHN_2)_{1\times1}$

Figure 1: Two hierarchical hypercube networks, HHN_1 and HHN_2.

4. MOLECULAR DESCRIPTORS FOR HIERARCHICAL HYPERCUBE NETWORKS HHN_1

In this section, we will consider the hierarchical hypercube network HHN_1, and then find their degree-based M-polynomials. By applying this M-polynomial we will investigate various kind of topological indices on this proposed structure.

Lemma 4.1: Let (HHN_1) be a hierarchical hypercube network then $M(\mathrm{HHN}_1;\ s_1,\ s_2)$ is

$$M(\mathrm{HHN}_1;\ s_1,\ s_2) = 16\, s_1^{\,2}\, s_2^{\,3} + 4\, s_1^{\,3}\, s_2^{\,3} + 24n\, s_1^{\,3}\, s_2^{\,3}$$

Proof: Let (HHN_1) be a hierarchical hypercube network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 16, & \alpha = 2,\ \beta = 3 \\ 24n + 4, & \alpha = 3,\ \beta = 3 \end{cases}$$

By applying the definition of M-polynomial, we have

$$M(\mathrm{HHN}_1;\ s_1,\ s_2) = \sum_{\alpha\le\beta} \rho(\alpha,\beta)\, s_1^{\,\alpha}\, s_2^{\,\beta}$$

$$= \sum_{2\le 3} \rho(2,3)\, s_1^{\,2}\, s_2^{\,3} + \sum_{3\le 3} \rho(3,3)\, s_1^{\,3}\, s_2^{\,3}$$

$$= (16)\, s_1^{\,2}\, s_2^{\,3} + (24n + 4)\, s_1^{\,3}\, s_2^{\,3}$$

$$= 16\, s_1^{\,2}\, s_2^{\,3} + 4\, s_1^{\,3}\, s_2^{\,3} + 24n\, s_1^{\,3}\, s_2^{\,3}$$

Theorem 4.2: Let (HHN_1) be a hierarchical hypercube network, then the topological indices are

$$
\begin{aligned}
M_1(\mathrm{HHN}_1) &= 104 + 144n \\
M_2(\mathrm{HHN}_1) &= 132 + 216n \\
{}^{m}M_2(\mathrm{HHN}_1) &= \frac{28}{9} + \frac{8n}{3} \\
R_\alpha(\mathrm{HHN}_1) &= 8\,n\,3^{\{2\,\alpha+3\}} + 2^{\{\alpha+5\}}3^{\{\alpha+1\}} + (4)\,9^{\{\alpha+1\}} \\
RR_\alpha(\mathrm{HHN}_1) &= 8\,n\,3^{\{-2\,\alpha-1\}} + 2^{\{3-\alpha\}}3^{\{-\alpha-1\}} + 4\,9^{\{-\alpha-1\}}
\end{aligned}
$$

Proof: Let (HHN_1) be a hierarchical hypercube network, the degree-based M-polynomial for (HHN_1) is

$$f(\mathcal{S}_1, \mathcal{S}_2) = 16\,\mathcal{S}_1{}^{2}\,\mathcal{S}_2{}^{3} + 4\,\mathcal{S}_1{}^{3}\,\mathcal{S}_2{}^{3} + 24n\,\mathcal{S}_1{}^{3}\,\mathcal{S}_2{}^{3}$$

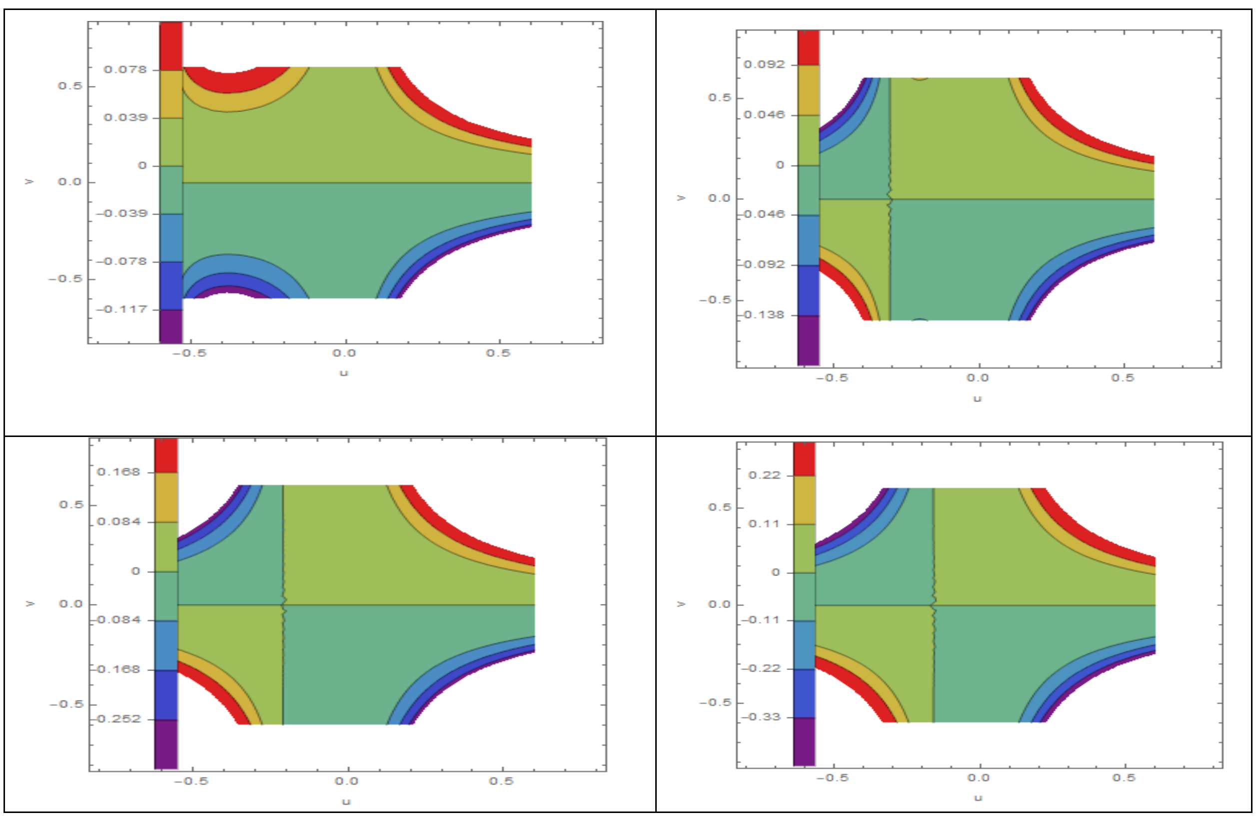


Figure 2: The graphical representation of M-polynomial (hierarchical hypercube network HHN_1) for $n = 1, 2, 3, 4$.

First of all we will calculate the required values to develop the desired topological indices

$$D_{\mathscr{S}_1} = \frac{\partial f(\mathscr{S}_1, \mathscr{S}_2)}{\partial \mathscr{S}_1} \mathscr{S}_1 = 32 \mathscr{S}_1{}^2 \mathscr{S}_2{}^3 + 12 \mathscr{S}_1{}^3 \mathscr{S}_2{}^3 + 72n \mathscr{S}_1{}^3 \mathscr{S}_2{}^3$$

$$D_{\mathscr{S}_2} = \frac{\partial f(\mathscr{S}_1, \mathscr{S}_2)}{\partial \mathscr{S}_1} \mathscr{S}_1 = 48 \mathscr{S}_1{}^2 \mathscr{S}_2{}^3 + 12 \mathscr{S}_1{}^3 \mathscr{S}_2{}^3 + 72n \mathscr{S}_1{}^3 \mathscr{S}_2{}^3$$

Table 4: Numerical comparison among computed topological indices for HHN_1.

n	M_1	M_2	${}^mM_2$	R_α	RR_α
1	248	348	5.77778	23868	0.112483
2	392	564	8.44444	41364	0.145405
3	536	780	11.1111	58860	0.178326
4	680	996	13.7778	76356	0.211248
5	824	1212	16.4444	93852	0.24417
6	968	1428	19.1111	111348	0.277092
7	1112	1644	21.7778	128844	0.310014
8	1256	1860	24.4444	146340	0.342936
9	1400	2076	27.1111	163836	0.375857
10	1544	2292	29.7778	181332	0.408779
11	1688	2508	32.4444	198828	0.441701
12	1832	2724	35.1111	216324	0.474623
13	1976	2940	37.7778	233820	0.507545
14	2120	3156	40.4444	251316	0.540466
15	2264	3372	43.1111	268812	0.573388
16	2408	3588	45.7778	286308	0.60631
17	2552	3804	48.4444	303804	0.639232
18	2696	4020	51.1111	321300	0.672154
19	2840	4236	53.7778	338796	0.705075
20	2984	4452	56.4444	356292	0.737997

$$D_{\mathscr{S}_1} D_{\mathscr{S}_2} = \mathscr{S}_1 \frac{\partial f(\mathscr{S}_1, \mathscr{S}_2)}{\partial \mathscr{S}_1} D_{\mathscr{S}_2} = 96 \mathscr{S}_1{}^2 \mathscr{S}_2{}^3 + 36 \mathscr{S}_1{}^3 \mathscr{S}_2{}^3 + 216n \mathscr{S}_1{}^3 \mathscr{S}_2{}^3$$

$$D^a_{\mathscr{S}_1} D^a_{\mathscr{S}_2} = 216\, n\, \mathscr{S}_1{}^3 \mathscr{S}_2{}^3 9^{\{\alpha\}} + 36\, \mathscr{S}_1{}^3 \mathscr{S}_2{}^3 9^{\{\alpha\}} + 96\, \mathscr{S}_1{}^2 \mathscr{S}_2{}^3 6^{\{\alpha\}}$$

$$\delta_{\mathscr{S}_2} = \int_0^{\mathscr{S}_2} \left(\frac{f(\mathscr{S}_1, t)}{t}\right) \mathfrak{D}t = \frac{16 \mathscr{S}_1{}^2 \mathscr{S}_2{}^3}{3} + \frac{4 \mathscr{S}_1{}^3 \mathscr{S}_2{}^3}{3} + 8n \mathscr{S}_1{}^3 \mathscr{S}_2{}^3$$

$$\delta_{\mathscr{S}_1} \delta_{\mathscr{S}_2} = \int_0^{\mathscr{S}_1} \left(\frac{\delta_{\mathscr{S}_2}}{t}\right) \mathfrak{D}t = \frac{8 \mathscr{S}_1{}^2 \mathscr{S}_2{}^3}{3} + \frac{4 \mathscr{S}_1{}^3 \mathscr{S}_2{}^3}{9} + \frac{8}{3} n \mathscr{S}_1{}^3 \mathscr{S}_2{}^3$$

$$M_1(\mathrm{HHN}_1) = \left[\left(D_{\mathscr{S}_1} + D_{\mathscr{S}_2}\left(M(G, \mathscr{S}_1, \mathscr{S}_2)\right)\right)\right] |_{(\mathscr{S}_1, \mathscr{S}_2)=(1,1)}$$

$$= 80\,\mathscr{s}_1^{\,2}\,\mathscr{s}_2^{\,3} + 24\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3} + 144n\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 104 + 144n$$

$$M_2(\mathrm{HHN}_1) = \left[\left(D_{\mathscr{s}_1} D_{\mathscr{s}_2}\left(M(G,\mathscr{s}_1,\,\mathscr{s}_2)\right)\right)\right]\,\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 96\,\mathscr{s}_1^{\,2}\,\mathscr{s}_2^{\,3} + 36\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3} + 216n\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 132 + 216n$$

$$^{m}M_2(\mathrm{HHN}_1) = \left[\left(S_{\mathscr{s}_1} S_{\mathscr{s}_2}\left(M(G,\qquad \mathscr{s}_1,\,\mathscr{s}_2)\right)\right)\right]\,\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= \frac{8\,\mathscr{s}_1^{\,2}\,\mathscr{s}_2^{\,3}}{3} + \frac{4\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}}{9} + \frac{8}{3}n\,\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= \frac{28}{9} + \frac{8n}{3}$$

$$R_\alpha(\mathrm{HHN}_1) = \left[\left(D^{\alpha}_{\mathscr{s}_1} D^{\alpha}_{\mathscr{s}_2}\left(M(G,\mathscr{s}_1,\,\mathscr{s}_2)\right)\right)\right]\,\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 216\,n\;\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}9^{\{\alpha\}} + 36\;\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}9^{\{\alpha\}} + 96\;\mathscr{s}_1^{\,2}\,\mathscr{s}_2^{\,3}6^{\{\alpha\}}\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 8\,n\,3^{\{2\,\alpha+3\}} + 2^{\{\alpha+5\}3^{\{\alpha+1\}}} + 4\,9^{\{\alpha+1\}}$$

$$RR_\alpha(\mathrm{HHN}_1) = \left[\left(S^{\alpha}_{\mathscr{s}_1} S^{\alpha}_{\mathscr{s}_2}\left(M(G,\mathscr{s}_1,\,\mathscr{s}_2)\right)\right)\right]\,\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= \frac{8\;\mathscr{s}_1^{\,2}\,\mathscr{s}_2^{\,3}}{3*6^{\alpha}} + \frac{4\;\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}}{9*9^{\alpha}} + \frac{8}{3*9^{\alpha}}n\;\mathscr{s}_1^{\,3}\,\mathscr{s}_2^{\,3}\big|_{(\mathscr{s}_1,\,\mathscr{s}_2)=(1,1)}$$

$$= 8\,n\,3^{\{-2\,\alpha-1\}} + 2^{\{3-\alpha\}3^{\{-\alpha-1\}}} + 4\,9^{\{-\alpha-1\}}$$

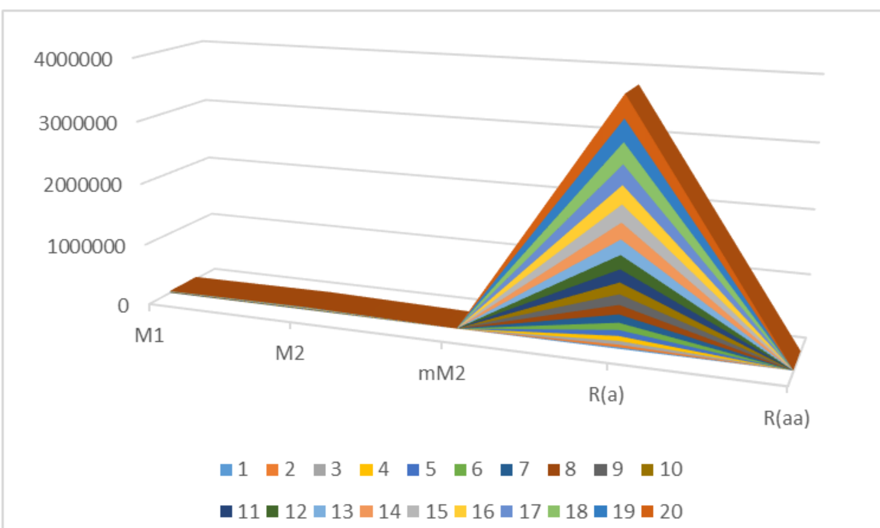


Figure 3: The graphical comparison of numeric values of Table 4.

Theorem 4.3: Let (HHN_1) be a hierarchical hypercube network, then the topological indices are

$$SSD_3(\mathrm{HHN}_1) = 696 + 1296n$$

$$SSD_5(\mathrm{HHN}_1) = \frac{128}{3} + 48n$$

$$I(\mathrm{HHN}_1) = \frac{116}{15} + 8n$$

$$H(\mathrm{HHN}_1) = 60 + 72n$$

$$F(\mathrm{HHN}_1) = 280 + 432n$$

Proof: Let (HHN_1) be a hierarchical hypercube network, the degree based M-polynomial for (HHN_1) is

$$f(\mathfrak{s}_1, \mathfrak{s}_2) = 16\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} + 4\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 24n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}$$

First of all we will calculate the required values to develop the desired topological indices

$$D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2} = 80\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} + 24\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 144n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}$$

$$D_{\mathfrak{s}_2}\left(D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2}\right) = 240\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} + 72\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 432n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}$$

$$D_{\mathfrak{s}_1}D_{\mathfrak{s}_2}\left(D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2}\right) = 480\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} + 216\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 1296n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}$$

$$SSD_3(\mathrm{HHN}_1)\,) = \left[D_{\mathfrak{s}_1}D_{\mathfrak{s}_2}\left(\left(D_{\mathfrak{s}_1} + D_{\mathfrak{s}_2}\right)\left(M(G, \mathfrak{s}_1, \mathfrak{s}_2)\right)\right)\right]\Big|_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$$

$$= 480\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} + 216\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 1296n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}\Big|_{(\mathfrak{s}_1, \mathfrak{s}_2)=(1,1)}$$

$$= 696 + 1296n$$

$$D_{\mathfrak{s}_1}\delta_{\mathfrak{s}_2} = \mathfrak{s}_1\frac{\partial}{\partial\,\mathfrak{s}_1}\left(\delta_{\mathfrak{s}_2}\right) = \frac{32\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3}}{3} + 4\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 24n$$

Similarly;

$$\delta_{\mathfrak{s}_1}D_{\mathfrak{s}_2} = \int_0^{\mathfrak{s}_1}\left(\frac{D_{\mathfrak{s}_2}}{t}\right)\mathfrak{D}t = 24\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3} +$$

$$4\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 24n\,\mathfrak{s}_1^{\,3}$$

$$D_{\mathfrak{s}_1}\delta_{\mathfrak{s}_2} + \delta_{\mathfrak{s}_1}D_{\mathfrak{s}_2} = \frac{104\,\mathfrak{s}_1^{\,2}\,\mathfrak{s}_2^{\,3}}{3} + 8\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3} + 48n\,\mathfrak{s}_1^{\,3}\,\mathfrak{s}_2^{\,3}$$

$$SSD_5(\mathrm{HHN}_1)) = \left[\left(S_{\delta_1}D_{\delta_1} + S_{\delta_2}D_{\delta_2}\left(M(G,\delta_1,\ \delta_2)\right)\right)\right]\ |_{(\delta_1,\delta_2)=(1,1)}$$
$$= \frac{104\ \delta_1{}^2\ \delta_2{}^3}{3} + 8\ \delta_1{}^3\ \delta_2{}^3 + 48n\ \delta_1{}^3\ \delta_2{}^3|_{(\delta_1,\delta_2)=(1,1)}$$
$$= \frac{128}{3} + 48n$$

The harmonic index is,

$$H(\mathrm{HHN}_1)) = \left[\left(2S_{\delta_1}J\left(M(G,\delta_1,\ \delta_2)\right)\right)\right]\ |_{(\delta_1,\delta_2)=(1,1)}$$
$$= \frac{32\ \delta_1{}^5}{5} + \frac{4\ \delta_1{}^6}{3} + 8n\ \delta_1{}^6|_{(\delta_1,\delta_2)=(1,1)}$$
$$= \frac{116}{15} + 8n$$

The inverse sum index is,

$$I(\mathrm{HHN}_1)) = \left[\left(S_{\delta_1}JD_{\delta_1}D_{\delta_2}\left(M(G,\delta_1,\ \delta_2)\right)\right)\right]\ |_{(\delta_1,\delta_2)=(1,1)}$$
$$= 48\ \delta_1{}^2\ \delta_2{}^3 + 12\ \delta_1{}^3\ \delta_2{}^3 + 72n\ \delta_1{}^3\ \delta_2{}^3|_{(\delta_1,\delta_2)=(1,1)}$$
$$= 60 + 72n$$
$$D_{\delta_1}^2 = 64\ \delta_1{}^2\ \delta_2{}^3 + 36\ \delta_1{}^3\ \delta_2{}^3 + 216n\ \delta_1{}^3\ \delta_2{}^3$$
$$D_{\delta_2}^2 = 144\ \delta_1{}^2\ \delta_2{}^3 + 36\ \delta_1{}^3\ \delta_2{}^3 + 216n\ \delta_1{}^3\ \delta_2{}^3$$

The forgotten topological index is,

$$F(\mathrm{HHN}_1)) = \left[(D_{\delta_1}{}^2 + D_{\delta_2}{}^2)\left(\left(M(G,\quad \delta_1,\ \delta_2)\right)\right)\right]\ |_{(\delta_1,\delta_2)=(1,1)}$$
$$= 208\ \delta_1{}^2\ \delta_2{}^3 + 72\ \delta_1{}^3\ \delta_2{}^3 + 432n\ \delta_1{}^3\ \delta_2{}^3|_{(\delta_1,\delta_2)=(1,1)}$$
$$= 280 + 432n$$

Table 5: Numerical comparison among computed topological indices for HHN_1.

n	SSD_3	SSD_5	H	I	F
1	1992	90.6667	15.7333	132	712
2	3288	138.667	23.7333	204	1144
3	4584	186.667	31.7333	276	1576
4	5880	234.667	39.7333	348	2008
5	7176	282.667	47.7333	420	2440

6	8472	330.667	55.7333	492	2872
7	9768	378.667	63.7333	564	3304
8	11064	426.667	71.7333	636	3736
9	12360	474.667	79.7333	708	4168
10	13656	522.667	87.7333	780	4600
11	14952	570.667	95.7333	852	5032
12	16248	618.667	103.733	924	5464
13	17544	666.667	111.733	996	5896
14	18840	714.667	119.733	1068	6328
15	20136	762.667	127.733	1140	6760
16	21432	810.667	135.733	1212	7192
17	22728	858.667	143.733	1284	7624
18	24024	906.667	151.733	1356	8056
19	25320	954.667	159.733	1428	8488
20	26616	1002.67	167.733	1500	8920

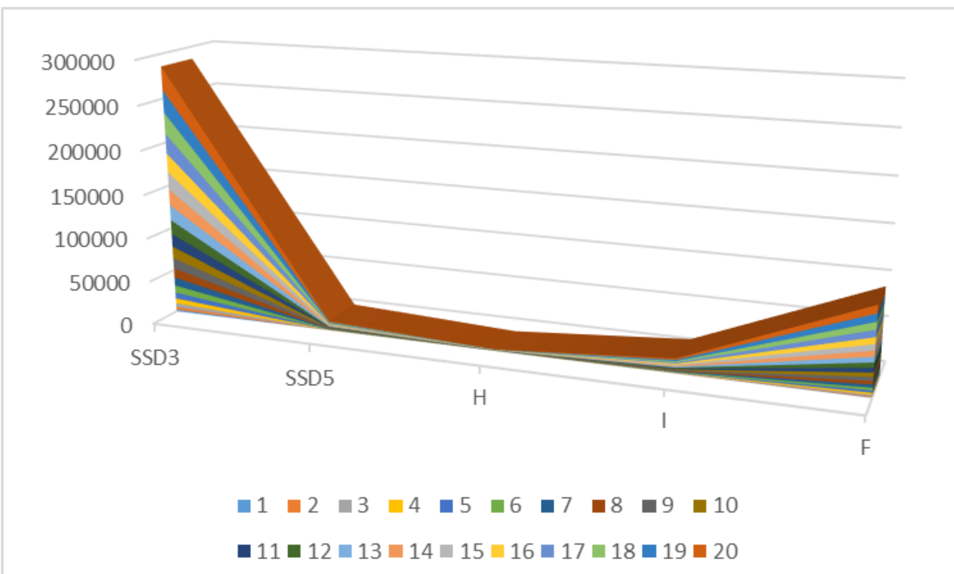


Figure 4: The graphical comparison of the numeric values of Table 5.

5. Molecular Descriptors for Hierarchical Hypercube Networks HHN_2

Lemma 5.1: Let (HHN_2) be a hierarchical hypercube network then $M(\mathrm{HHN}_2;\ \mathscr{s}_1,\ \mathscr{s}_2)$ is

$$M(\mathrm{HHN}_2;\ \mathscr{s}_1,\ \mathscr{s}_2) = 24\ \mathscr{s}_1{}^3\ \mathscr{s}_2{}^4 + 4\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4 + 32n\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4$$

Proof: Let (HHN_2) be a hierarchical hypercube network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 24, & \alpha = 3,\ \beta = 4 \\ 32n + 4, & \alpha = 4,\ \beta = 4 \end{cases}$$

By applying the definition of M-polynomial, we have

$$M(\mathrm{HHN}_2;\ \mathscr{s}_1,\ \mathscr{s}_2) = \sum_{\alpha\le\beta} \rho(\alpha,\beta)\ \mathscr{s}_1{}^{\alpha}\ \mathscr{s}_2{}^{\beta}$$

$$= \sum_{3\le 4} \rho(3,4)\ \mathscr{s}_1{}^3\ \mathscr{s}_2{}^4 + \sum_{4\le 4} \rho(4,4)\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4$$

$$= (24)\ \mathscr{s}_1{}^3\ \mathscr{s}_2{}^4 + (32n + 4)\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4$$

$$= 24\ \mathscr{s}_1{}^3\ \mathscr{s}_2{}^4 + 4\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4 + 32n\ \mathscr{s}_1{}^4\ \mathscr{s}_2{}^4$$

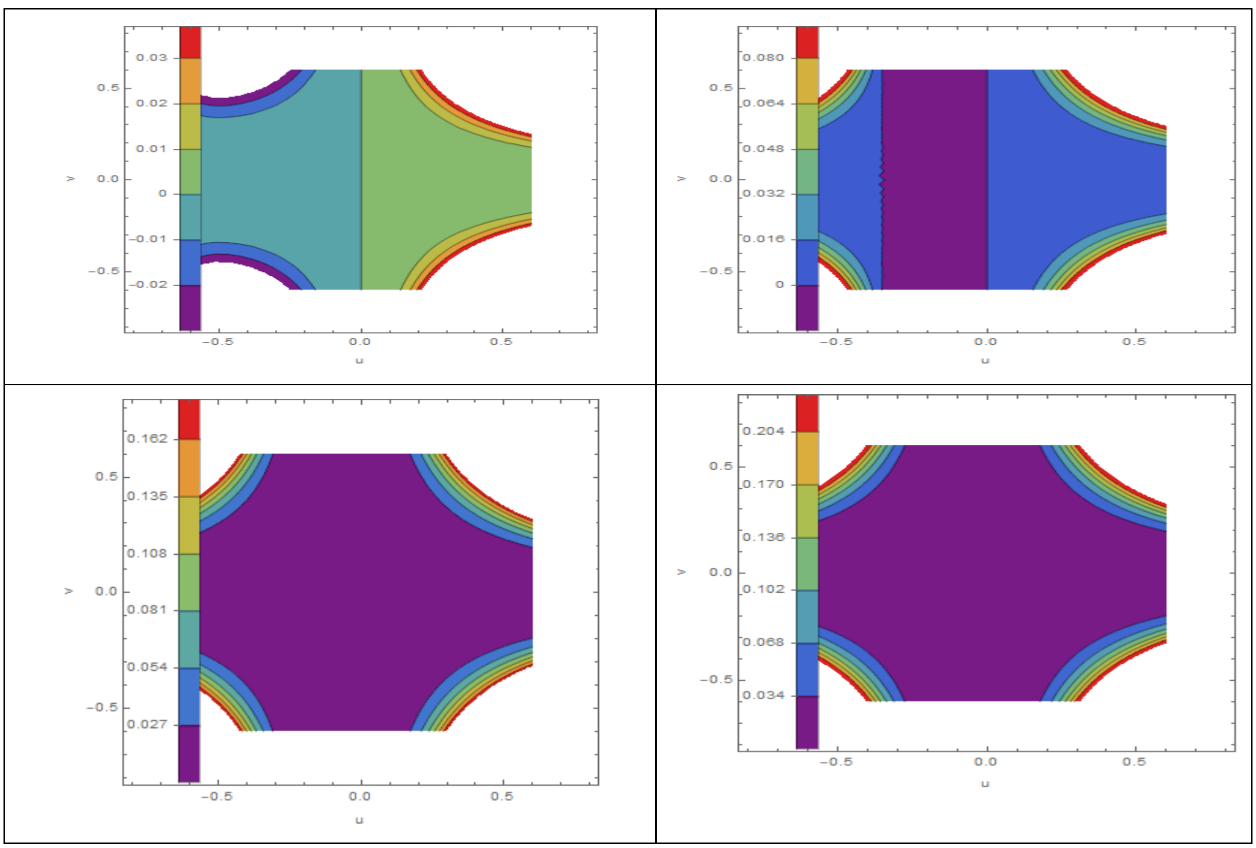


Figure 5: The graphical representation of M-polynomial (hierarchical hypercube network HHN_1) for $n = 1, 2, 3, 4$.

Theorem 5.2: Let (HHN_1) be a hierarchical hypercube network, then the topological indices are

$$M_1(HHN_2) = 200 + 256n$$
$$M_2(HHN_2) = 352 + 512n$$
$$^mM_2(HHN_2) = \frac{9}{4} + 2n$$
$$R_\alpha(HHN_2) = n\,2^{\{4\alpha+9\}} + 2^{\{2\alpha+5\}}3^{\{\alpha+2\}} + 4^{\{2\alpha+3\}}$$
$$RR_\alpha(HHN_2) = n\,2^{\{-4\alpha-3\}} + 2^{\{-2\alpha-1\}}3^{\{-\alpha-1\}} + 4^{\{-2\alpha-3\}}$$

Proof: Let (HHN_1) be a hierarchical hypercube network, the degree based M-polynomial for (HHN_2) is

$$f(\mathcal{S}_1, \mathcal{S}_2) = 24\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 4\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 32n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

First of all we will calculate the required values to develop the desired topological indices

$$D_{\mathcal{S}_1} = \frac{\partial f(\mathcal{S}_1, \mathcal{S}_2)}{\partial \mathcal{S}_1}\,\mathcal{S}_1 = 72\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 16\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 128n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

$$D_{\mathcal{S}_2} = \frac{\partial f(\mathcal{S}_1, \mathcal{S}_2)}{\partial \mathcal{S}_1}\,\mathcal{S}_1 = 96\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 16\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 128n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

$$D_{\mathcal{S}_1}D_{\mathcal{S}_2} = \mathcal{S}_1\frac{\partial f(\mathcal{S}_1, \mathcal{S}_2)}{\partial \mathcal{S}_1}\,D_{\mathcal{S}_2} = 288\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 64\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 512n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

$$D_{\mathcal{S}_1}^{a}D_{\mathcal{S}_2}^{a} = 512\,n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}16^{\{\alpha\}} + 64\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}16^{\{\alpha\}} + 288\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4}12^{\{\alpha\}}$$

$$\delta_{\mathcal{S}_2} = \int_0^{\mathcal{S}_2}\left(\frac{f(\mathcal{S}_1, t)}{t}\right)\mathfrak{D}t = 6\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + \mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 8n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

$$\delta_{\mathcal{S}_1}\delta_{\mathcal{S}_2} = \int_0^{\mathcal{S}_1}\left(\frac{\delta_{\mathcal{S}_2}}{t}\right)\mathfrak{D}t = 2\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + \frac{\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}}{4} + 2n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}$$

$$(HHN_2) = \left[\left(D_{\mathcal{S}_1} + D_{\mathcal{S}_2}\left(M(G, \mathcal{S}_1, \mathcal{S}_2)\right)\right)\right]\,|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 168\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 32\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 256n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 200 + 256n$$

$$M_2(HHN_2) = \left[\left(D_{\mathcal{S}_1}D_{\mathcal{S}_2}\left(M(G, \mathcal{S}_1, \mathcal{S}_2)\right)\right)\right]\,|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 288\,\mathcal{S}_1^{\,3}\mathcal{S}_2^{\,4} + 64\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4} + 512n\,\mathcal{S}_1^{\,4}\mathcal{S}_2^{\,4}|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 352 + 512n$$

$$^mM_2(HHN_2) = \left[\left(S_{\mathcal{S}_1}S_{\mathcal{S}_2}\left(M(G, \mathcal{S}_1, \mathcal{S}_2)\right)\right)\right]\,|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 2\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + \frac{\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4}{4} + 2n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= \frac{9}{4} + 2n$$

$$R_\alpha(\mathrm{HHN}_2) = \left[\left(D^\alpha_{\mathcal{S}_1} D^\alpha_{\mathcal{S}_2}\left(M(G,\mathcal{S}_1,\,\mathcal{S}_2)\right)\right)\right]\,|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 512\,n\;\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 16^{\{\alpha\}} + 64\;\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 16^{\{\alpha\}} + 288\;\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 12^{\{\alpha\}}|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}\,.$$

$$= n\,2^{\{4\,\alpha+9\}} + 2^{\{2\,\alpha+5\}}3^{\{\alpha+2\}} + 4^{\{2\,\alpha+3\}}$$

$$RR_\alpha\,(\mathrm{HHN}_2) = \left[\left(S^\alpha_{\mathcal{S}_1} S^\alpha_{\mathcal{S}_2}\left(M(G,\mathcal{S}_1,\,\mathcal{S}_2)\right)\right)\right]\,|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= \frac{\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4}{6*12^\alpha} + \frac{\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4}{64*16^\alpha} + \frac{1}{8*16^\alpha}n\;\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= n\,2^{\{-4\,\alpha-3\}} + 2^{\{-2\,\alpha-1\}}3^{\{-\alpha-1\}} + 4^{\{-2\,\alpha-3\}}$$

Table 6: Numerical comparison among computed topological indices for HHN_2.

n	M_1	M_2	$^mM_2$	R_α	RR_α
1	456	864	4.25	188928	0.00170672
2	712	1376	6.25	320000	0.00219501
3	968	1888	8.25	451072	0.00268329
4	1224	2400	10.25	582144	0.00317157
5	1480	2912	12.25	713216	0.00365985
6	1736	3424	14.25	844288	0.00414813
7	1992	3936	16.25	975360	0.00463641
8	2248	4448	18.25	1106432	0.00512469
9	2504	4960	20.25	1237504	0.00561297
10	2760	5472	22.25	1368576	0.00610126
11	3016	5984	24.25	1499648	0.00658954
12	3272	6496	26.25	1630720	0.00707782
13	3528	7008	28.25	1761792	0.0075661
14	3784	7520	30.25	1892864	0.00805438
15	4040	8032	32.25	2023936	0.00854266
16	4296	8544	34.25	2155008	0.00903094
17	4552	9056	36.25	2286080	0.00951922
18	4808	9568	38.25	2417152	0.0100075
19	5064	10080	40.25	2548224	0.0104958
20	5320	10592	42.25	2679296	0.0109841

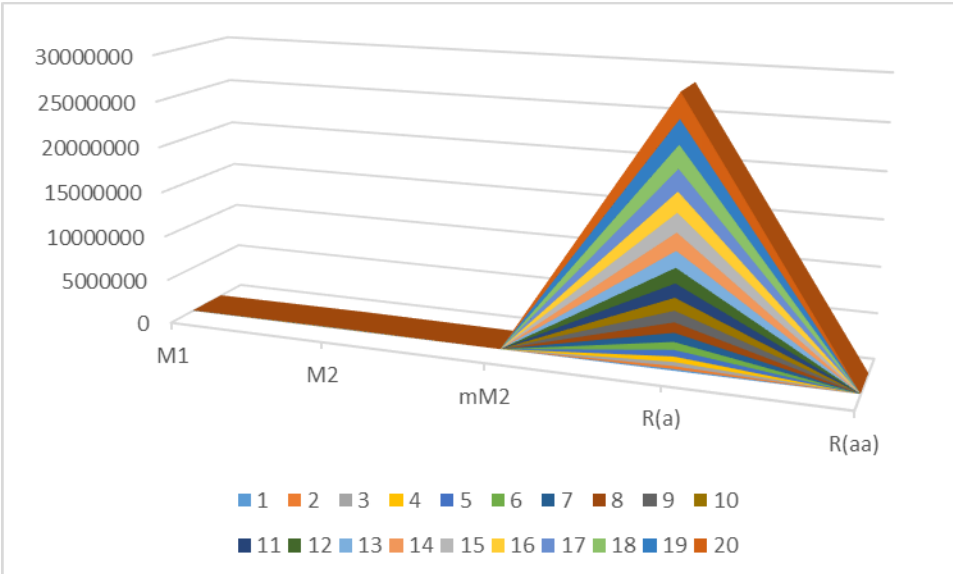


Figure 6: The graphical comparison of the numeric values of Table 6.

Theorem 5.3: Let (HHN_2) be a hierarchical hypercube network, then the topological indices are

$$SSD_3(\mathrm{HHN}_2) = 2528 + 4096n$$

$$SSD_5(\mathrm{HHN}_2) = 58 + 64n$$

$$I(\mathrm{HHN}_2) = \frac{55}{7} + 8n$$

$$H(\mathrm{HHN}_2) = 112 + 128n$$

$$F(\mathrm{HHN}_2) = 728 + 1024n$$

Proof: Let (HHN_2) be a hierarchical hypercube network, the degree based M-polynomial for (HHN_2) is

$$f(\mathcal{S}_1, \mathcal{S}_2) = 16\,\mathcal{S}_1^{\,2}\,\mathcal{S}_2^{\,3} + 4\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,3} + 24n\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,3}$$

First of all we will calculate the required values to develop the desired topological indices

$$D_{\mathcal{S}_1} + D_{\mathcal{S}_2} = 168\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,4} + 32\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4} + 256n\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4}$$

$$D_{\mathcal{S}_2}\left(D_{\mathcal{S}_1} + D_{\mathcal{S}_2}\right) = 672\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,4} + 128\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4} + 1024n\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4}$$

$$D_{\mathcal{S}_1}D_{\mathcal{S}_2}\left(D_{\mathcal{S}_1} + D_{\mathcal{S}_2}\right) = 2016\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,4} + 512\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4} + 4096n\,\mathcal{S}_1^{\,4}\,\mathcal{S}_2^{\,4}$$

$$SSD_3(\mathrm{HHN}_2)\,) = \left[D_{\mathcal{S}_1}D_{\mathcal{S}_2}\left(\left(D_{\mathcal{S}_1} + D_{\mathcal{S}_2}\right)\left(M(G,\mathcal{S}_1, \mathcal{S}_2)\right)\right)\right] \Big|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 480\,\mathcal{S}_1^{\,2}\,\mathcal{S}_2^{\,3} + 216\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,3} + 1296n\,\mathcal{S}_1^{\,3}\,\mathcal{S}_2^{\,3}\Big|_{(\mathcal{S}_1, \mathcal{S}_2)=(1,1)}$$

$$= 2528 + 4096n$$

$$D_{\mathcal{S}_1}\delta_{\mathcal{S}_2} = \mathcal{S}_1 \frac{\partial}{\partial \mathcal{S}_1}\left(\delta_{\mathcal{S}_2}\right) = 32\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 4\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 32n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4$$

Similarly;

$$\delta_{\mathcal{S}_1}D_{\mathcal{S}_2} = \int_0^{\mathcal{S}_1}\left(\frac{D_{\mathcal{S}_2}}{t}\right)\mathfrak{D}t = 18\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 4\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 32n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4$$

By the addition

$$D_{\mathcal{S}_1}\delta_{\mathcal{S}_2} + \delta_{\mathcal{S}_1}D_{\mathcal{S}_2} = 50\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 8\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 64n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4$$

$$SSD_5(\mathrm{HHN}_2)) = \left[\left(S_{\mathcal{S}_1}D_{\mathcal{S}_1} + S_{\mathcal{S}_2}D_{\mathcal{S}_2}\left(M(G,\mathcal{S}_1,\ \mathcal{S}_2)\right)\right)\right]\ |_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 50\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 8\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 64n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 58 + 64n$$

The harmonic index is,

$$H(\mathrm{HHN}_2)) = \left[\left(2S_{\mathcal{S}_1}J\left(M(G,\mathcal{S}_1,\ \mathcal{S}_2)\right)\right)\right]\ |_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= \frac{48\,\mathcal{S}_1{}^7}{7} + \mathcal{S}_1{}^8 + 8n\,\mathcal{S}_1{}^8|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= \frac{55}{7} + 8n$$

The inverse sum index is,

$$I(\mathrm{HHN}_2)) = \left[\left(S_{\mathcal{S}_1}JD_{\mathcal{S}_1}D_{\mathcal{S}_2}\left(M(G,\mathcal{S}_1,\ \mathcal{S}_2)\right)\right)\right]\ |_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 96\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 16\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 128n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 112 + 128n$$

$$D^2_{\mathcal{S}_1} = 216\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 64\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 512n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4$$

$$D^2_{\mathcal{S}_2} = 384\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 64\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 512n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4$$

The forgotten topological index is,

$$F(\mathrm{HHN}_2)) = \left[(D_{\mathcal{S}_1}{}^2 + D_{\mathcal{S}_2}{}^2)\left(\left(M(G,\mathcal{S}_1,\ \mathcal{S}_2)\right)\right)\right]\ |_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 600\,\mathcal{S}_1{}^3\,\mathcal{S}_2{}^4 + 128\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4 + 1024n\,\mathcal{S}_1{}^4\,\mathcal{S}_2{}^4|_{(\mathcal{S}_1,\mathcal{S}_2)=(1,1)}$$

$$= 728 + 1024n$$

Table 7: Numerical comparison among computed topological indices for HHN_2.

n	SSD_3	SSD_5	H	I	F
1	6624	122	15.8571	240	1752
2	10720	186	23.8571	368	2776
3	14816	250	31.8571	496	3800
4	18912	314	39.8571	624	4824
5	23008	378	47.8571	752	5848
6	27104	442	55.8571	880	6872
7	31200	506	63.8571	1008	7896
8	35296	570	71.8571	1136	8920
9	39392	634	79.8571	1264	9944
10	43488	698	87.8571	1392	10968
11	47584	762	95.8571	1520	11992
12	51680	826	103.857	1648	13016
13	55776	890	111.857	1776	14040
14	59872	954	119.857	1904	15064
15	63968	1018	127.857	2032	16088
16	68064	1082	135.857	2160	17112
17	72160	1146	143.857	2288	18136
18	76256	1210	151.857	2416	19160
19	80352	1274	159.857	2544	20184
20	84448	1338	167.857	2672	21208

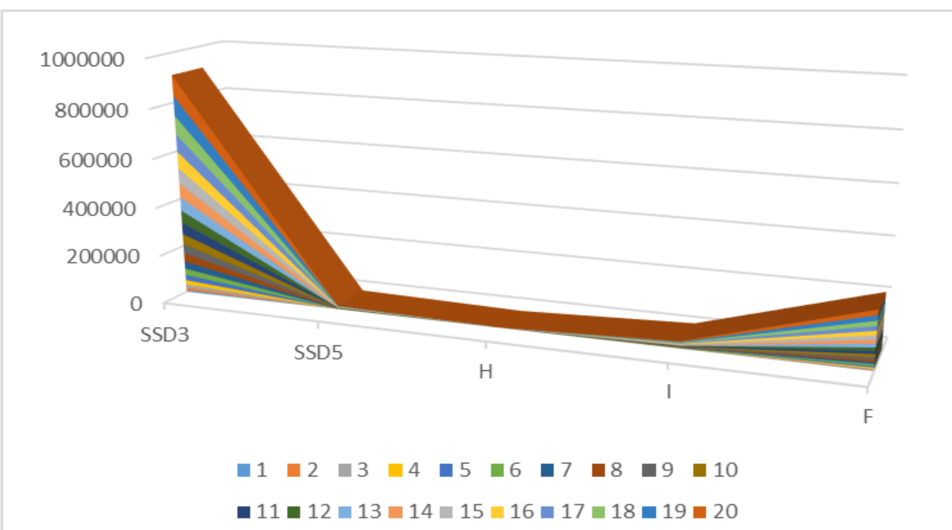


Figure 7: The graphical comparison of the numeric values of Table 7.

6. MOLECULAR DEGREES-BASED ENTROPIES FOR HIERARCHICAL HYPERCUBE NETWORKS

Lemma 6.1: Let (HHN_1) be a hierarchical hypercube network, then we have

$$RZE_1(\mathrm{HHN}_1) = 16 + 16n$$
$$RZE_2(\mathrm{HHN}_1) = \frac{126}{5} + 36n$$

Proof: Let (HHN-1) be a hierarchical hypercube network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 16, & \alpha = 2,\ \beta = 3 \\ 24n + 4, & \alpha = 3,\ \beta = 3 \end{cases}$$

$$RZE_1(\mathrm{HHN}_1) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}} = (16)\frac{5}{6} + (24n+4)\frac{6}{9} = 16 + 16n$$

$$RZE_2(\mathrm{HHN}_1) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}} = (16)\frac{6}{5} + (24n+4)\frac{9}{6} = \frac{126}{5} + 36n$$

Proposition 6.2. Let (HHN_1) be a hierarchical hypercube network, then we have

$$\boldsymbol{ENT}_{\boldsymbol{RZE_1}}(\mathrm{HHN}_1) = \mathrm{Log}[16\,(1+\mathrm{n})] - \frac{\mathrm{Log}\left[1220703125\ 3^{-16\,(1+\mathrm{n})}5^{\frac{1}{3}}65536^{3\,(1+\mathrm{n})}(1+6\,\mathrm{n})^{\frac{8}{3}+16\,\mathrm{n}}\right]}{16\,(1+\mathrm{n})}$$

$$\boldsymbol{ENT}_{\boldsymbol{RZE_2}}(\mathrm{HHN}_1) = \frac{Log[5] + 5\,Log[19073486328125]}{18\,(7+10\,n)}$$
$$\frac{-5\,Log\left[3^{\frac{126}{5}+36\,n}64^{17+6\,n}(1+6\,n)^{6+36\,n}\right] + 18\,(7+10\,n)Log\left[\frac{126}{5}+36\,n\right]}{18\,(7+10\,n)}$$

Proposition 6.3. Let (HHN_1) be a hierarchical hypercube network, then we have

$$RZE_1(\mathrm{HHN}_1) = 16 + 16n$$
$$RZE_2(\mathrm{HHN}_1) = \frac{344}{7} + 64n$$

Proof: Let (HHN_2) be a hierarchical hypercube network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 24, & \alpha = 3,\ \beta = 4 \\ 32n + 4, & \alpha = 4,\ \beta = 4 \end{cases}$$

$$RZE_1(\mathrm{HHN}_2) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}} = (24)\frac{7}{12} + (32n+4)\frac{8}{16} = 16 + 16n$$

$$RZE_2(\mathrm{HHN}_2) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}} = (24)\frac{12}{7} + (32n+4)\frac{16}{8} = \frac{344}{7} + 64n$$

Proposition 6.4. Let (HHN_1) be a hierarchical hypercube network, then we have

$$\boldsymbol{ENT_{RZE_1}}(\mathrm{HHN}\ \ ) = \mathrm{Log}[16\,(1+\mathrm{n})] - \frac{\mathrm{Log}[678223072849\ 65536^{1+\mathrm{n}}(1+8\,\mathrm{n})^{2+16\,\mathrm{n}}]}{16\,(1+\mathrm{n})}$$

$$\boldsymbol{ENT_{RZE_2}}(\mathrm{HHN}_2) = Log\left[\frac{344}{7} + 64\,n\right] - \left(\frac{7\,Log\left[\frac{1330279464729113309844748891857449678409\ 2^{\frac{1608}{7}+192\,n}3^{\frac{2}{7}}(1+8\,n)^{8+64\,n}}{44567640326363195900190045974568007\ 7^{\frac{1}{7}}}\right]}{8\,(43+56\,n)}\right)$$

7. CONCLUSION

The M-polynomial framework has been applied to the study of Hierarchical Hypercube Networks (HHNs) in this paper and it has proved to be a reliable tool in the analysis and study of complex network structures as a coherent and unified approach. Using the natural symmetry of HHNs and their recursive properties, we obtained closed form expressions of their M-polynomials that provide very accurate degree distributions of such networks. The resulting general forms are used to greatly simplify the calculation of a large number of degree-based topological indices. Certain significant degree-based topological indices were estimated with the use of these M-polynomials, which gave quantitative value of the structural complexity of HHNs. These indices can provide useful information on the possible physicochemical attributes and functional attributes of such networks and hence the applicability of the chemical graph theory tools in the study of hierarchies and symmetries structures. The visual representations of the M-polynomials also helped to improve the comprehension of the structural behavior of HHNs by providing the clear visual representation of the degree correlations in the networks. In general, the findings validate that M-polynomial method is an efficient and strong means of analyzing the Hierarchical Hypercube

Networks and other nanostructured systems based on it. This technique can be applied to other classes of interconnection networks and molecular graphs to open up the future research on structural characterization and prediction of properties of complex chemical and computational networks.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

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