Study of topology of block shift networks via topological indices

Murat Cancan¹ orcid.org/0000-0002-8606-2274

Iftikhar Ahmad² orcid.org/0000-0001-5879-5801

Sarfaz Ahmad³

¹Van Yznc Yil University, Faculty of Education, Van, Turkey.

m_cencen@yahoo.com

²COMSATS University Islamabad, Dept. of Mathematics, Lahore, Pakistan.

iffi6301@gmail.com

³COMSATS University Islamabad, Dept. of Mathematics, Lahore, Pakistan.

iffi6301@gmail.com

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Abstract:

Topological indices (TIs) are important numerical number associate with the molecular graph of a chemical structure/compound because due to these parameters, one can guess almost all properties of concerned structure/compound with our performing experiments. In recent years, huge amount work has been done for calculating degree-dependent indices for different structures/compounds. In order to compute TIs, one need to do many calculations. Our aim of this paper is to present a simple method to compute degree-dependent TIs. We computed M-polynomials for Block Shift Networks and with the help of this simple algebraic polynomials, we recovered nine important TIs for Block Shift Networks. Our work is important for chemists, physicians and pharmaceutical industry.

Keywords: Topological index; Physical properties of compounds; Graph; Network.

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1. Introduction

The representation of a chemical structure with the help of TIs is an interesting topic in chemistry and bio-informatics [8]. This approach help us in deciding properties of chemical compounds without performing experiments [8]. TIs in this way an important tool for chemists and mathematician are interesting in computing TIs of different chemical structures [1]. The first topological index was Wiener index defined in 1947 [29]. After the success of this index [13,30], Randic index (RI) was defined in [24]. The formula for RI is:

$$R_{-\frac{1}{2}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

This is the most successful index till now and has been studied extensively [24,25]. Zagreb indices (ZIs) are also oldest TIs and the first ZI and second ZI are defined in [12] as:

$$M_1(G) = \sum_{uv \in E(G)} d_u + d_v$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

For details about applications of these indices, we refer [4,16,23,25,27,28].

The formula for the redefined ZI [18] is:

$${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

The mathematical formula for the symmetric division index (SDI) [11] is:

$$SDI(G) = \sum_{uv \in E(G)} \left\{ \frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}} + \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} \right\}.$$

Other interesting TIs is harmonic index (HI) [6] which is a variant of RI and mathematical formula for this TI is:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u d_v}.$$

The other two TIs of our interest are inverse sum index (ISI) [2] and Augmented ZI [7] and these TIs are defined as:

$$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v},$$

and

$$A(G) = \sum_{uv \in E(G)} \left\{ \frac{d_u d_v}{d_u + d_v - 2} \right\}^3.$$

The above defined TIs are important for the researcher working in chemistry [3.5.14.15.17.22.23.26] and huge computational work is required for calculating these indices [10,22]. In order to reduce computational work [30], M-polynomial has been introduced and one can get almost every degree-dependent index from this simple polynomial [20,27]. The mathematical formula of this polynomial is

$$M(G; x, y) = \sum_{uv \in E(G)} (x^{d_u} y^{d_v}).$$

The relation of this polynomial with above mentioned nine TIs can be found in [21,22].

In this paper, our aim is to compute M-polynomial for Block-Shift Network.

The Block shift network $BSN - 1$ is the shuffle-exchange network n -dimensional hypercube, while block shift network $BSN - 2$ is the complete network, as shown in Figure 1.1 and Figure 1.2 respectively. Let G be a block shift network. It can be seen from Figure 1 that the number of vertices and edges in $(BSN - 1)$ are $16a^2$ and $24a^2 - 2$ respectively. From Figure 2, one can observe that the number of vertices and edges in $(BSN - 2)$ are $16a^2$ and $32a^2 - 2$ respectively.

Figure 1.1: $(BSN - 1)_{(3 \times 3)}$ Figure 1.2: $(BSN - 2)_{(1 \times 1)}$

2. Main Results

In this section, we compute M-polynomials of understudy networks and recover nine TIs from these polynomials.

2.1. Results for $(BSN - 1)_{(n \times n)}$

Theorem 2.1. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3.$$

Proof. The $(BSN - 1)_{(n \times n)}$ network has following two type of edges based on the degree of end vertices:

$$E_{\{2,3\}}((BSN - 1)_{(n \times n)}) = \{uv \in E((BSN - 1)_{(n \times n)}) : d_u = 2, d_v = 3\},$$

$$E_{\{3,3\}}((BSN - 1)_{(n \times n)}) = \{uv \in E((BSN - 1)_{(n \times n)}) : d_u = 3, d_v = 3\},$$

such that

$$|E_{\{2,3\}}((BSN - 1)_{(n \times n)})| = 8,$$

$$|E_{\{3,3\}}((BSN - 1)_{(n \times n)})| = (24n^2 - 10),$$

Now from the definition of M-polynomial, we have

$$\begin{aligned} M(G; x, y) &= \sum_{\delta \leq i \leq j \leq \Delta} m_{ij} x^i y^j \\ &= \sum_{2 \leq 3} m_{23} x^2 y^3 + \sum_{3 \leq 3} m_{33} x^3 y^3 \\ &= |E_{\{2,3\}}((BSN - 1)_{(n \times n)})| x^2 y^3 + |E_{\{3,3\}}((BSN - 1)_{(n \times n)})| x^3 y^3 \\ &= 8x^2 y^3 + (24n^2 - 10) x^3 y^3. \end{aligned}$$

□

Corollary 2.2. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$M_1((BSN - 1)_{(n \times n)}) = 144n^2 - 20$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2 y^3 + (24n^2 - 10) x^3 y^3$.

Then

$$D_x(f(x, y)) = 16x^2 y^3 + 3(24n^2 - 10) x^3 y^3,$$

$$D_y(f(x, y)) = 24x^2 y^3 + 3(24n^2 - 10) x^3 y^3.$$

Hence

$$\begin{aligned} M_1((BSN - 1)_{(n \times n)}) &= D_x f + D_y f \Big|_{x=y=1} \\ &= 144n^2 - 20. \end{aligned}$$

□

Corollary 2.3. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$M_2((BSN - 1)_{(n \times n)}) = 216n^2 - 42$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$D_y(f(x, y)) = 24x^2y^3 + 3(24n^2 - 10)x^3y^3,$$

$$D_x D_y(f(x, y)) = 48x^2y^3 + 9(24n^2 - 10)x^3y^3,$$

Hence

$$\begin{aligned} M_2((BSN - 1)_{(n \times n)}) &= D_x D_y f \Big|_{x=y=1} \\ &= 216n^2 - 42. \end{aligned}$$

□

Corollary 2.4. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$${}^m M_2((BSN - 1)_{(n \times n)}) = \frac{8n^2}{3} + \frac{2}{9}$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$S_y(f(x, y)) = \frac{8x^2y^3}{3} + \frac{(24n^2 - 10)x^3y^3}{3},$$

$$S_x S_y(f(x, y)) = \frac{4x^2y^3}{3} + \frac{(24n^2 - 10)x^3y^3}{9}.$$

Hence

$$\begin{aligned} {}^m M_2((BSN - 1)_{(n \times n)}) &= S_x S_y f \Big|_{x=y=1} \\ &= \frac{8n^2}{3} + \frac{2}{9}. \end{aligned}$$

□

Corollary 2.5. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$R_\alpha((BSN - 1)_{(n \times n)}) = 24^\alpha 2^\alpha + 3^{2\alpha} (24n^2 - 10)$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$D_y^\alpha(f(x, y)) = 24^\alpha x^2 y^3 + 3^\alpha (24n^2 - 10) x^3 y^3.$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 24^\alpha 2^\alpha x^2 y^3 + 3^{2\alpha} (24n^2 - 10) x^3 y^3.$$

Hence

$$\begin{aligned} R_\alpha((BSN - 1)_{(n \times n)}) &= D_x^\alpha D_y^\alpha f \Big|_{x=y=1} \\ &= 24^\alpha 2^\alpha + 3^{2\alpha} (24n^2 - 10). \end{aligned}$$

□

Corollary 2.6. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$RR_\alpha((BSN - 1)_{(n \times n)}) = \frac{8^\alpha}{3^\alpha 2^\alpha} + \frac{24n^2 - 10}{3^{2\alpha}}$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$S_y^\alpha(f(x, y)) = \frac{8^\alpha x^2 y^3}{3^\alpha} + \frac{(24n^2 - 10)x^3 y^3}{3^\alpha}.$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = \frac{8^\alpha x^2 y^3}{3^\alpha 2^\alpha} + \frac{(24n^2 - 10)x^3 y^3}{3^\alpha 3^\alpha}.$$

Hence

$$\begin{aligned} RR_\alpha((BSN - 1)_{(n \times n)}) &= S_x^\alpha S_y^\alpha f \Big|_{x=y=1} \\ &= \frac{8^\alpha}{3^\alpha 2^\alpha} + \frac{(24n^2 - 10)}{3^{2\alpha}}. \end{aligned}$$

□

Corollary 2.7. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$SSD((BSN - 1)_{(n \times n)}) = \frac{52}{3} + 2(24n^2 - 10)$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$S_x D_y(f(x, y)) = 12x^2y^3 + (24n^2 - 10)x^3y^3,$$

$$D_x S_y(f(x, y)) = \frac{16x^2y^3}{3} + (24n^2 - 10)x^3y^3.$$

Hence

$$\begin{aligned} SSD((BSN - 1)_{(n \times n)}) &= (D_x S_y f + S_x D_y f) \Big|_{x=y=1} \\ &= \frac{52}{3} + 2(24n^2 - 10). \end{aligned}$$

□

Corollary 2.8. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$H((BSN - 1)_{(n \times n)}) = 2 \left(\frac{8}{5} + \frac{(24n^2 - 10)}{6} \right)$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$J(f(x, y)) = 8x^5 + (24n^2 - 10)x^6,$$

$$2S_x J(f(x, y)) = 2\left(\frac{8x^5}{5} + \frac{(24n^2 - 10)x^6}{6}\right).$$

Hence

$$\begin{aligned} H((BSN - 1)_{(n \times n)}) &= 2S_x Jf \Big|_{x=1} \\ &= 2\left(\frac{8}{5} + \frac{(24n^2 - 10)}{6}\right). \end{aligned}$$

□

Corollary 2.9. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$I((BSN - 1)_{(n \times n)}) = \frac{48}{5} + \frac{3(24n^2 - 10)}{2}$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$\begin{aligned} D_y(f(x, y)) &= 24x^2y^3 + 3(24n^2 - 10)x^3y^3, \\ D_x D_y(f(x, y)) &= 48x^2y^3 + 9(24n^2 - 10)x^3y^3, \\ J D_x D_y(f(x, y)) &= 48x^5 + 9(24n^2 - 10)x^6, \\ S_x J D_x D_y(f(x, y)) &= \frac{48x^5}{5} + \frac{9x^6(24n^2 - 10)}{6}. \end{aligned}$$

Hence

$$\begin{aligned} I((BSN - 1)_{(n \times n)}) &= S_x J D_x D_y f \Big|_{x=1} \\ &= \frac{48}{5} + \frac{3(24n^2 - 10)}{2}. \end{aligned}$$

□

Corollary 2.10. Let $(BSN - 1)_{(n \times n)}$ be the block shift Network, then

$$A((BSN - 1)_{(n \times n)}) = \frac{2187n^2}{8} - \frac{1597}{32}$$

Proof. Let $f(x, y) = M(G; x, y) = 8x^2y^3 + (24n^2 - 10)x^3y^3$.

Then

$$D_y^3(f(x, y)) = 216x^2y^3 + 27(24n^2 - 10)x^3y^3,$$

$$\begin{aligned}
 D_x^3 D_y^3 (f(x, y)) &= 1728x^2y^3 + 729(24n^2 - 10)x^3y^3, \\
 JD_x^3 D_y^3 (f(x, y)) &= 1728x^5 + 729(24n^2 - 10)x^6, \\
 Q_{-2} JD_x^3 D_y^3 (f(x, y)) &= 1728x^3 + 729(24n^2 - 10)x^4, \\
 S_x^3 Q_{-2} JD_x^3 D_y^3 (f(x, y)) &= 64x^2 + \frac{729x^4(24n^2 - 10)}{64}.
 \end{aligned}$$

Hence

$$\begin{aligned}
 A((BSN - 1)_{(n \times n)}) &= S_x^3 Q_{-2} JD_x^3 D_y^3 f \Big|_{x=1} \\
 &= \frac{2187n^2}{8} - \frac{1597}{32}.
 \end{aligned}$$

□

2.2. Results for $(BSN - 2)_{(n \times n)}$

Theorem 2.11. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4.$$

Proof. The $(BSN - 2)_{(n \times n)}$ network has following two type of edges based on the degree of end vertices:

$$E_{\{3,4\}}((BSN - 2)_{(n \times n)}) = \{uv \in E((BSN - 2)_{(n \times n)}) : d_u = 3, d_v = 4\},$$

$$E_{\{4,4\}}((BSN - 2)_{(n \times n)}) = \{uv \in E((BSN - 2)_{(n \times n)}) : d_u = 4, d_v = 4\},$$

such that

$$|E_{\{3,4\}}((BSN - 2)_{(n \times n)})| = 12,$$

$$|E_{\{4,4\}}((BSN - 2)_{(n \times n)})| = (32n^2 - 14),$$

Now from the definition of M-polynomial, we have

$$\begin{aligned}
 M(G; x, y) &= \sum_{\delta \leq i \leq j \leq \Delta} m_{ij} x^i y^j \\
 &= \sum_{3 \leq 4} m_{34} x^3 y^4 + \sum_{4 \leq 4} m_{44} x^4 y^4 \\
 &= |E_{\{3,4\}}((BSN - 2)_{(n \times n)})| x^3 y^4 + |E_{\{4,4\}}((BSN - 2)_{(n \times n)})| x^4 y^4 \\
 &= 12x^3y^4 + (32n^2 - 14)x^4y^4.
 \end{aligned}$$

□

Corollary 2.12. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$M_1((BSN - 2)_{(n \times n)}) = 256n^2 - 28$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$D_x(f(x, y)) = 36x^3y^4 + 4(32n^2 - 14)x^4y^4,$$

$$D_y(f(x, y)) = 48x^3y^4 + 4(32n^2 - 14)x^4y^4.$$

Hence

$$\begin{aligned} M_1((BSN - 2)_{(n \times n)}) &= D_x f + D_y f \Big|_{x=y=1} \\ &= 256n^2 - 28. \end{aligned}$$

□

Corollary 2.13. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$M_2((BSN - 2)_{(n \times n)}) = 512n^2 - 80$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$D_y(f(x, y)) = 48x^3y^4 + 4(32n^2 - 14)x^4y^4,$$

$$D_x D_y(f(x, y)) = 144x^3y^4 + 16(32n^2 - 14)x^4y^4,$$

Hence

$$\begin{aligned} M_2((BSN - 2)_{(n \times n)}) &= D_x D_y f \Big|_{x=y=1} \\ &= 512n^2 - 80. \end{aligned}$$

□

Corollary 2.14. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$${}^m M_2((BSN - 2)_{(n \times n)}) = 2n^2 + \frac{1}{8}$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$S_y(f(x, y)) = 3x^3y^4 + \frac{(32n^2 - 14)x^4y^4}{4},$$

$$S_x S_y(f(x, y)) = x^3y^4 + \frac{(32n^2 - 14)x^4y^4}{16}.$$

Hence

$$\begin{aligned} {}^m M_2((BSN - 2)_{(n \times n)}) &= S_x S_y f \Big|_{x=y=1} \\ &= 2n^2 + \frac{1}{8}. \end{aligned}$$

□

Corollary 2.15. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$R_\alpha((BSN - 2)_{(n \times n)}) = 48^\alpha 3^\alpha + 4^{2\alpha} (32n^2 - 14)$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$D_y^\alpha(f(x, y)) = 48^\alpha x^3y^4 + 4^\alpha (32n^2 - 14)x^4y^4.$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 48^\alpha 3^\alpha x^3y^4 + 4^{2\alpha} (32n^2 - 14)x^4y^4.$$

Hence

$$\begin{aligned} R_\alpha((BSN - 2)_{(n \times n)}) &= D_x^\alpha D_y^\alpha f \Big|_{x=y=1} \\ &= 48^\alpha 3^\alpha + 4^{2\alpha} (32n^2 - 14). \end{aligned}$$

□

Corollary 2.16. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$RR_\alpha((BSN - 2)_{(n \times n)}) = 1 + \frac{32n^2 - 14}{4^{2\alpha}}.$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$S_y^\alpha(f(x, y)) = 3^\alpha x^3y^4 + \frac{(32n^2 - 14)x^4y^4}{4^\alpha},$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = x^3y^4 + \frac{(32n^2 - 14)x^4y^4}{4^{2\alpha}}.$$

Hence

$$\begin{aligned} RR_\alpha((BSN - 2)_{(n \times n)}) &= S_x^\alpha S_y^\alpha f \Big|_{x=y=1} \\ &= 1 + \frac{32n^2 - 14}{4^{2\alpha}}. \end{aligned}$$

□

Corollary 2.17. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$SSD((BSN - 2)_{(n \times n)}) = 64n^2 - 3$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$S_x D_y (f(x, y)) = 16x^3y^4 + (32n^2 - 14)x^4y^4,$$

$$D_x S_y (f(x, y)) = 9x^3y^4 + (32n^2 - 14)x^4y^4.$$

Hence

$$\begin{aligned} SSD \left((BSN - 2)_{(n \times n)} \right) &= (D_x S_y f + S_x D_y f) \Big|_{x=y=1} \\ &= 64n^2 - 3. \end{aligned}$$

□

Corollary 2.18. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$H \left((BSN - 2)_{(n \times n)} \right) = 2 \left(\frac{12}{7} + \frac{(32n^2 - 14)}{8} \right)$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$J(f(x, y)) = 12x^7 + (32n^2 - 14)x^8,$$

$$2S_x J(f(x, y)) = 2 \left(\frac{12x^7}{7} + \frac{(32n^2 - 14)x^8}{8} \right).$$

Hence

$$\begin{aligned} H \left((BSN - 2)_{(n \times n)} \right) &= 2S_x Jf \Big|_{x=1} \\ &= 2 \left(\frac{12}{7} + \frac{(32n^2 - 14)}{8} \right). \end{aligned}$$

□

Corollary 2.19. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$I \left((BSN - 2)_{(n \times n)} \right) = 64n^2 - \frac{52}{7}$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$D_y(f(x, y)) = 48x^3y^4 + 4(32n^2 - 14)x^4y^4,$$

$$D_x D_y(f(x, y)) = 144x^3y^4 + 16(32n^2 - 14)x^4y^4,$$

$$J D_x D_y(f(x, y)) = 144x^7 + 16(32n^2 - 14)x^8,$$

$$S_x J D_x D_y (f(x, y)) = \frac{144x^7}{7} + 2x^8 (32n^2 - 14).$$

Hence

$$\begin{aligned} I \left((BSN - 2)_{(n \times n)} \right) &= S_x J D_x D_y f \Big|_{x=1} \\ &= 64n^2 - \frac{52}{7}. \end{aligned}$$

□

Corollary 2.20. Let $(BSN - 2)_{(n \times n)}$ be the block shift Network, then

$$A \left((BSN - 2)_{(n \times n)} \right) = \frac{16384n^2}{27} - \frac{336128}{3375}$$

Proof. Let $f(x, y) = M(G; x, y) = 12x^3y^4 + (32n^2 - 14)x^4y^4$.

Then

$$\begin{aligned} D_y^3 (f(x, y)) &= 768x^3y^4 + 64(32n^2 - 14)x^4y^4, \\ D_x^3 D_y^3 (f(x, y)) &= 20736x^3y^4 + 4096(32n^2 - 14)x^4y^4, \\ J D_x^3 D_y^3 (f(x, y)) &= 20736x^7 + 4096(32n^2 - 14)x^8, \\ Q_{-2} J D_x^3 D_y^3 (f(x, y)) &= 20736x^5 + 4096(32n^2 - 14)x^6, \\ S_x^3 Q_{-2} J D_x^3 D_y^3 (f(x, y)) &= \frac{20736x^5}{125} + \frac{512x^6(32n^2 - 14)}{27}. \end{aligned}$$

Hence

$$\begin{aligned} A \left((BSN - 2)_{(n \times n)} \right) &= S_x^3 Q_{-2} J D_x^3 D_y^3 f \Big|_{x=1} \\ &= \frac{16384n^2}{27} - \frac{336128}{3375}. \end{aligned}$$

□

Conclusion

In this paper, we computed several degree-dependent indices for Block Shift Networks. We used edge division for this purpose and with the help of our results, one can guess the properties for Block Shift Networks.

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