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Computation of Distance Matrices of Primary Subgraphs

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Abstract

The graph-theoretical (topological) distance matrices and their invariants (polynomials, spectra and wiener numbers) are presented. Use of distance matrix and its invariants in chemistry is surveyed. Method used to compute distance polynomials is Le Verrier-Faddeev-Frame method.Along with this, Wiener numbers are computed. Some new results are presented.

Keywords: Distance Matrix, Spectrum, Wiener number, Distance Polynomials, Le Verrier-Faddeev-Frame method.

1. Introduction

Mathematical chemistry and chemical graph theory both were developing deliberately with only a few bounds until the 1970's. Then a number of research groups appeared that commenced to flourish chemical graph theory, speedily. One of the directions in which this forceful renaissance was progressing was the graph-theoretical matrices.

Matrices are the pillars of chemical graph theory. And distance matrix is such a mathematical tool which is being a lot of used in chemistry [1–7] in graph- theoretical(topological) [8–10]. versions. The distance matrix has found a great importance in other areas such as in applied mathematics [11–15,15,17–19], physics [20–22] or chemistry [4] and sociology [23], computer science [24], economics [25] etc. Firstly, distance matrix was introduced by Brunel [26] in uncompleted form. However, the origins of distance matrix are found in the first paper of Cayley [27].

Distance matrix is used in both implicit and explicit forms [4] in chemistry. Clark and Kettle [28] in 1975, were the first who have implicitly used distance matrix in chemistry. They have utilized the distance matrix for examining the permutational isomers of stereochemically nonrigid molecules. These writers have determined that shortest path sequence which is mandatory to effect the rearrangement and because of this, they have told the difference between the various interconversion mechanisms for pairs of permutational isomers. These paths were utilized in the formation of relevant distance matrix. Now the condition is almost changed after the expertly written Rouvray's articles [2,4,29] and Balban's [30], King's [31] and Trinajstic's [3,8,32] well known books on chemical graph theory. Instead of all this ,there's a necessity of a basic origin of enlightenment in literature on the topics of topological and topographic distance matrices, their invariants and applications.

Also in explicit form, distance matrix is used to obtain the distance polynomials and distance spectra of variety of molecular structures [7,33–35]. Although, the implicit utilization of distance matrix in chemistry, was not popular in early stage but some work in this area was done by Wiener [36] in 1947. His work was to adumbrate the physical properties of alkanes by developing a structure-property model. In sake of this, Wiener mentioned the path number just as a numerical characteristics of molecule. He done all this very cleverly. Path number be defined as the sum of the distances between any two carbon atoms in alkanes in terms of the carbon-carbon bonds. Wiener also mentioned polarity number and he given its definition as the number of couples of carbon atoms splitted up by three carbon-carbon bonds. By practicing the linear combination of path and polarity number's, Wiener was capable to guess the boiling points of alkanes [36] and that was a fair prediction. In the privilege of the wiener's contribution in determining number of paths in molecule structures, term "Wiener number" or "Wiener index" has been given to the number of distances in all chemical structures. Hosoya [28] was first who determined a connection between the distance matrix and Wiener number. He find out that "the half sum of the elements of the distance matrix is actually equal to the wiener number".

The distance matrix is playing a role of a pioneer for obtaining novel topological as well as topographic indices. It become evident today the most significant uses of distance matrix in chemistry [2,4,29,37–39].

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2. Methods

Modified form of Le Verrier-Faddeev-Frame (LVFF) method is used for computations in this paper. Once the matrix is converted into tridiagonal form, so that the eigen values could be directly read. Firstly, find the distance spectrum of G, as the collection of eigen values of the distance matrix is known as the distance spectrum of graph G. For the order of mbym distance matrix, the coefficients c_m in the LVFF method can be computed by

$$c_m = \frac{1}{m}\sum_{i=1}^{m}(D_m)_{ii}$$

where the matrix D_m is given by,

$$(D_m)_{ii} = D_{ii}(B_m)_{ii}$$

In above expression, D shows distance matrix and B_m is an auxiliary matrix defined as,

$$(B_m)_{ii} = (D_m)_{ii} - (c_m I)_{ii}$$

The above is an iterative procedure which ends when the B-matrix vanishes, i.e. when m = M:

$$(B_M)_{ii} = (D_M)_{ii} - (c_M I)_{ii} = 0$$

. After this, the result is the distance polynomial of given graph G which is;

$$\delta(G;x) = c_0 x^M - \sum_{m=1}^{M} c_m x^{M-m}$$

And the Wiener number is also computed by using the formula given by Wiener, which is "the half sum of the elements of the distance matrix is actually equal to the wiener number".

3. Main Results

The main objective of the study is to enhance the application of Le Verrier-Faddeev-Frame method up to some more structures in Chemistry. And to include some new structures with proves in this area. To widened the use of distance matrix in Chemistry.

Theorem 3.1. *Distance Polynomial for the graph G_1 is $\delta(G;x) = x^6 - 65x^4 - 295x^3 - 503.9916x^2 - 351.9848x - 79.992$.*

Proof. Distance matrix of G_1 is:

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 2 & 2 \\ 1 & 0 & 2 & 2 & 1 & 1 \\ 1 & 2 & 0 & 2 & 3 & 3 \\ 1 & 2 & 2 & 0 & 3 & 3 \\ 2 & 1 & 3 & 3 & 0 & 2 \\ 2 & 1 & 3 & 3 & 2 & 0 \end{pmatrix}$$

1)Distance spectrum:

$$\{-4.5616, -2, -2, -1, -0.4384, 10\}$$

2)

$$\sum_{i=1}^{6}(D_{ii}) = \sum_{i=1}^{6}(D_1)_{ii} = 0$$

$$c_1 = 0$$

3)

$$\{(B_1)_{ii} = (D_1)_{ii} - (c_1 I)_{ii}\}_{i=1,2,\ldots,6} = \{-4.5616, -2, -2, -1, -0.4384, 10\}$$

$$(D_2)_{ii} = (D)_{ii}(B_1)_{ii} = \{20.8082, 4, 4, 1, 0.1922, 100\}$$

$$c_2 = \frac{1}{2}\sum_{i=1}^{6}(D_2)_{ii} = \frac{1}{2}(130.0004) = 65.0002$$

4)

$$\{(B_2)_{ii} \quad = \quad (D_2)_{ii} - (c_2 I)_{ii}\}_{i=1,2,\ldots,6}$$

$$= \{-44.192, -61.0002, -61.0002, -64.0002, -64.808, 34.9998\}$$

$$(D_3)_{ii} = (D)_{ii}(B_2)_{ii} = \{201.5862, 122.0004, 122.0004, 64.0002, 28.4118, 349.998\}$$

$$c_3 = \frac{1}{3}(887.997) = 295.999$$

5)

$$\begin{aligned} \{(B_3)_{ii} &= (D_3)_{ii} - (c_3 I)_{ii}\}_{i=1,2,\ldots,6} \\ &= \{-94.4128, -173.9986, -173.9986, -231.9988, -267.5872, 53.999\} \end{aligned}$$

$$(D_4)_{ii} = (D)_{ii}(B_3)_{ii} = \{430.6734, 347.9972, 347.9972, 231.9988, 117.3102, 539.99\}$$

$$c_4 = \frac{1}{4}(2015.9664) = 503.9916$$

6)

$$\begin{aligned} \{(B_4)_{ii} &= (D_4)_{ii} - (c_4 I)_{ii}\}_{i=1,2,\ldots,6} \\ &= \{-73.3182, -155.9944, -155.9944, -271.9928, -386.6814, 35.9984\} \end{aligned}$$

$$(D_5)_{ii} = (D)_{ii}(B_4)_{ii} = \{334.4483, 311.9888, 311.9888, 271.9928, 169.5211, 359.984\}$$

$$c_5 = \frac{1}{5}(1759.9238) = 351.9848$$

7)

$$\begin{aligned} \{(B_5)_{ii} &= (D_5)_{ii} - (c_5 I)_{ii}\}_{i=1,2,\ldots,6} \\ &= \{-17.5365, -39.996, -39.996, -79.992, -182.4637, 7.9992\} \end{aligned}$$

$$(D_6) = (D)_{ii}(B_5)_{ii} = \{79.9945, 79.992, 79.992, 79.992, 79.992, 79.992\}$$

$$c_6 = \frac{1}{6}(479.952) = 79.992$$

8)

$$\begin{aligned} \{(B_6)_{ii} &= (D_6)_{ii} - (c_6 I)_{ii}\}_{i=1,2,\ldots,6} \\ &= \{0, 0, 0, 0, 0, 0\} \end{aligned}$$

So, distance polynomial of given graph G is; $\delta(G; x) = x^6 - 65x^4 - 295x^3 - 503.9916x^2 - 351.9848x - 79.992$. ☐

Corollary 3.1. *The Wiener index $W(G)$ of a graph G is;*

$$W(G) = \frac{1}{2}\sum_l \sum_m (D)_{lm} = \frac{1}{2}(58) = 29.$$

Theorem 3.2. *Distance Polynomial for the graph G_2 is $\delta(G; x) = x^7 - 87.9998x^5 - 485.9994x^4 - 994.0062x^3 - 892.0495x^2 - 336.2912x - 44.4756$.*

Proof. Distance matrix of G_2 is:

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 2 & 3 & 3 \\ 1 & 0 & 1 & 2 & 1 & 2 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ 3 & 2 & 1 & 0 & 3 & 3 & 2 \\ 2 & 1 & 2 & 3 & 0 & 1 & 2 \\ 3 & 2 & 2 & 3 & 1 & 0 & 1 \\ 3 & 2 & 1 & 2 & 2 & 1 & 0 \end{pmatrix}$$

1) Distance spectrum=$\{-4.2143, -4.1381, -1.4608, -1.2013, -0.3337, -0.3249, 11.7171\}$ 2)

$$\sum_{i=1}^{7}(D)_{ii} = \sum_{i=1}^{7}(D_1)_{ii} = 0$$

$$c_1 = 0$$

3)

$$\{(B_1)_{ii} = (D_1)_{ii} - (c_1 I)\}_{i=1,2,\ldots,7}$$

$$= \{-4.2143, -4.1381, -1.4608, -1.2013, -0.3337, -0.3249, 11.7171\}$$

$$(D_2)_{ii} = (D)_{ii}(B_1)_{ii} = \{17.7603, 17.1239, 2.1339, 1.4431, 0.1426, 0.1055, 137.2904\}$$

$$c_2 = \frac{1}{2}(175.9997) = 87.9998$$

4)

$$\begin{aligned} \{(B_2)_{ii} &= (D_2)_{ii} - (c_2 I)\}_{i=1,2,\ldots,7} \\ &= \{-70.2395, -70.8759, -85.8659, -86.5567, -87.8572, -87.8943, 49.2906\} \end{aligned}$$

$$\begin{aligned} (D_3)_{ii} &= (D)_{ii}(B_2)_{ii} \\ &= \{296.0103, 293.2915, 125.4329, 103.9805, 33.1836, 28.5568, 577.5428\} \end{aligned}$$

$$c_3 = \frac{1}{3}(1457.9984) = 485.9994$$

5)

$$\begin{aligned} \{(B_3)_{ii} &= (D_3)_{ii} - (c_3 I)\}_{i=1,2,\ldots,7} \\ &= \{-189.9891, -192.7079, -360.5665, -382.0189, -452.8158, -457.4426, 91.5434\} \end{aligned}$$

$$\begin{aligned} (D_4)_{ii} &= (D)_{ii}(B_3)_{ii} \\ &= \{800.6710, 797.4445, 526.7155, 458.9193, 171.0285, 148.6231, 1072.6231\} \end{aligned}$$

$$c_4 = \frac{1}{4}(3976.025) = 994.0062$$

6)

$$\begin{aligned} \{(B_4)_{ii} &= (D_4)_{ii} - (c_4 I)\}_{i=1,2,\ldots,7} \\ &= \{-193.3352, -196.5617, -467.2907, -535.0869, -822.9777, -845.3831, 78.6169\} \end{aligned}$$

$$\begin{aligned} (D_5)_{ii} &= (D)_{ii}(B_5)_{ii} \\ &= \{814.7725, 813.3919, 682.6182, 642.7998, 310.8386, 274.6649, 921.1620\} \end{aligned}$$

$$c_5 = \frac{1}{5}(4460.2479) = 892.0495$$

7)

$$\begin{aligned} \{(B_5)_{ii} &= (D_5)_{ii} - (c_5 I)\}_{i=1,2,\ldots,7} \\ &= \{-77.277, -78.6576, -209.4313, -249.2497, -581.2109, -617.3846, 29.1125\} \end{aligned}$$

$$\begin{aligned} (D_6)_{ii} &= (D)_{ii}(B_6)_{ii} \\ &= \{325.6684, 325.4930, 305.9372, 299.4236, 219.5233, 200.5882, 341.1140\} \end{aligned}$$

$$c_6 = \frac{1}{6}(2017.7477) = 336.2912$$

8)

$$\begin{aligned} \{(B_6)_{ii} &= (D_6)_{ii} - (c_6 I)\}_{i=1,2,\ldots,7} \\ &= \{-10.6228, -10.8612, -30.354, -36.8676, -116.7679, -135.703, 3.8338\} \end{aligned}$$

$$\begin{aligned} (D_7)_{ii} &= (D)_{ii}(B_7)_{ii} \\ &= \{44.7676, 44.9447, 44.3411, 44.2890, 44.1032, 44.0899, 44.7921\} \end{aligned}$$

$$c_7 = \frac{1}{7}(311.3276) = 44.4756$$

9)

$$\begin{aligned} \{(B_7)_{ii} &= (D_7)_{ii} - (c_7 I)\}_{i=1,2,\ldots,7} \\ &= \{0, 0, 0, 0, 0, 0, 0\} \end{aligned}$$

So, distance polynomial of given graph G is; $\delta(G; x) = x^7 - 87.9998x^5 - 485.9994x^4 - 994.0062x^3 - 892.0495x^2 - 336.2912x - 44.4756$. □

Corollary 3.2. *The Wiener index $W(G)$ of graph G is;*

$$W(G) = \frac{1}{2}\sum_{l}\sum_{m}(D)_{lm} = \frac{1}{2}(80) = 40.$$

Theorem 3.3. *Distance Polynomial for graph G_3 is $\delta(G; x) = x^8 - 0x^7 - 127.00048207x^6 - 800.00052110x^5 - 1880.97512458x^4 - 2007.90895706x^3 - 1000.89542577x^2 - 215.956357249x - 15.994$.*

Proof. Distance matrix of G_3 is:

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 3 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 3 & 2 \\ 2 & 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ 3 & 3 & 2 & 1 & 0 & 1 & 2 & 2 \\ 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 3 & 2 & 2 & 1 & 0 & 1 \\ 1 & 2 & 2 & 1 & 2 & 2 & 1 & 0 \end{pmatrix}$$

1) Distance spectrum=

$$\{-6.3723, -3.7321, -1.7957, -1, -0.6277, -0.2679, -0.1596, 13.9553\}$$

2)

$$\sum_{i=1}^{8}(D)_{ii} = \sum_{i=1}^{8}(D_1)_{ii} = 0$$
$$c_1 = 0$$

3)

$$\begin{aligned} \{(B_1)_{ii} &= (D_1)_{ii} - (c_1 I)\}_{i=1,2,\ldots,8} \\ &= \{-6.3723, -3.7321, -1.7957, -1, -0.6277, -0.2679, -0.1596, 13.9553\} \end{aligned}$$

$$\begin{aligned} (D_2)_{ii} &= (D)_{ii}(B_1)_{ii} \\ &= \{40.60620729, 13.92857041, 3.22453849, 1, 0.39400729, 0.07177041, \\ &\quad 0.02547216, 194.75039809\} \end{aligned}$$

$$c_2 = \frac{1}{2}(254.00096414) = 127.00048207$$

4)

$$\begin{aligned} \{(B_2)_{ii} &= (D_2)_{ii} - (c_2 I)\}_{i=1,2,\ldots,8} \\ &= \{-86.39427478, -113.07191166, -123.77594358, -126.00048207, \\ &\quad -126.60647478, -126.92871166, -126.97500991, 67.74991602\} \end{aligned}$$

$$\begin{aligned} (D_3)_{ii} &= (D)_{ii}(B_2)_{ii} \\ &= \{550.530237181, 421.995681506, 222.264461887, 126.00048107, \\ &\quad 79.47088421, 34.00420185, 20.26521158, 945.47043034\} \end{aligned}$$

$$c_3 = \frac{1}{3}(2400.00156331) = 800.00052110$$

5)

$$\begin{aligned} \{(B_3)_{ii} &= (D_3)_{ii} - (c_3 I)\}_{i=1,2,\ldots,8} \\ &= \{-249.47028392, -378.0048396, -577.73605921, -674.00003903, \\ &\quad -720.52963689, -765.99631925, -779.73530952, 145.46988193\} \end{aligned}$$

$$\begin{aligned} (D_4)_{ii} &= (D)_{ii}(B_3)_{ii} \\ &= \{1589.69949022, 1410.75186187, 1037.44064152, 674.00003903, \end{aligned}$$

$$452.27645307, 205.21041392, 124.44575539, 2030.0758433\}$$

$$c_4 = \frac{1}{4}(7523.90049832) = 1880.97512458$$

6)

$$\begin{aligned}\{(B_4)_{ii} &= (D_4)_{ii} - (c_4 I)\}_{i=1,2,\ldots,8} \\ &= \{-291.27563436, -470.22326271, -843.53448306, -1206.97508528, \\ &\quad -1428.69867151, -1675.76471066, -1756.52936919, 149.10071842\}\end{aligned}$$

$$\begin{aligned}(D_5)_{ii} &= (D)_{ii}(B_4)_{ii} \\ &= \{1856.09572483, 1754.92023876, 1514.73487123, 1206.97508528, \\ &\quad 896.794156107, 448.937365986, 280.342087323, 2080.74525577\}\end{aligned}$$

$$c_5 = \frac{1}{5}(10039.5447853) = 2007.90895706$$

7)

$$\begin{aligned}\{(B_5)_{ii} &= (D_5)_{ii} - (c_5 I)\}_{i=1,2,\ldots,8} \\ &= \{-151.81323223, -252.9887183, -493.17408583, -800.93387178, \\ &\quad -1111.11480095, -1558.97159107, -1727.56686974, 72.83629871\}\end{aligned}$$

$$\begin{aligned}(D_6)_{ii} &= (D)_{ii}(B_5)_{ii} \\ &= \{967.399459739, 944.179195567, 885.592705925, 800.93387178, \\ &\quad 697.446760556, 417.648489248, 275.719672411, 1016.45239939\}\end{aligned}$$

$$c_6 = \frac{1}{6}(6005.37255462) = 1000.89542577$$

8)

$$\begin{aligned}\{(B_6)_{ii} &= (D_6)_{ii} - (c_6 I)\}_{i=1,2,\ldots,8} \\ &= \{-33.495966031, -56.716230203, -115.302719845, -199.96155399, \\ &\quad -303.448665214, -583.246936522, -725.175753359, 15.55697362\}\end{aligned}$$

$$\begin{aligned}(D_7)_{ii} &= (D)_{ii}(B_6)_{ii} \\ &= \{213.446344339, 211.670642741, 207.049094026, 199.96155399, \\ &\quad 190.474727155, 156.251854294, 115.738050236, 217.102233959\}\end{aligned}$$

$$c_7 = \frac{1}{7}(1511.69450074) = 215.956357241$$

9)

$$\begin{aligned}\{(B_7)_{ii} &= (D_7)_{ii} - (c_7 I)\}_{i=1,2,\ldots,8} \\ &= \{-2.51001291, -4.285714508, -8.907263223, -15.994803259, \\ &\quad -25.481630094, -59.704502955, -100.218307013, 1.14587671\}\end{aligned}$$

$$\begin{aligned}(D_8)_{ii} &= (D)_{ii}(B_7)_{ii} \\ &= \{15.9945552664, 15.9947151153, 15.9947725695, 15.994803259, \\ &\quad 15.99481921, 15.9948363416, 15.9948417993, 15.9910532511\}\end{aligned}$$

$$c_8 = \frac{1}{8}(127.954396812) = 15.994$$

10)

$$\begin{aligned}\{(B_8)_{ii} &= (D_8)_{ii} - (c_8 I)\}_{i=1,2,\ldots,8} \\ &= \{0, 0, 0, 0, 0, 0, 0, 0\}\end{aligned}$$

So, distance polynomial of given graph G is; $\delta(G; x) = x^8 - 0x^7 - 127.00048207x^6 - 800.00052110x^5 - 1880.97512458x^4 - 2007.90895706x^3 - 1000.89542577x^2 - 215.956357249x - 15.994.$ □

Corollary 3.3. *The Wiener index $W(G)$ of graph G is;*

$$W(G) = \frac{1}{2}\sum_{l}\sum_{m}(D)_{lm} = \frac{1}{2}(110) = 55.$$

4. Conclusions

In this paper we gave the graph-theoretical (topological) distance matrices and their invariants (polynomials, spectra and wiener numbers).And some new results of primary subgraphs are presented here.

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