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Original Scientific Paper

On the Detour Matrix*

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»We dance round in a ring and suppose,
But the Secret sits in the middle and knows.«

Robert Frost[1]

The detour matrix of a graph and its invariants (polynomial, spectrum and Wiener-like index) are discussed. Methods for computing these quantities are presented. Some comparisons with the distance matrix of a graph are given.

The detour matrix is briefly mentioned and defined by Buckley and Harary in their book on the distance in graphs.[2] Harary also delivered a talk on this matrix in the Department of Marine Sciences at The Texas A&M University in Galveston on April 4th, 1994. This talk stimulated us to report our work on the detour matrix, its polynomial and spectrum.

Definition of the detour matrix

The detour matrix $\Delta = \Delta(G)$ of a labeled connected graph G is a real symmetric $N \times N$ matrix whose (i,j)-entry is the length of the longest path from vertex i to vertex j. This definition is just opposite to the definition of the traditional distance matrix, often used in the (chemical) graph theory, whose entries are the shortest paths

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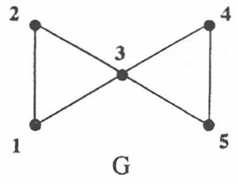
between the vertices in the graph.[1, 3–9] It is evident that the distance matrix and the detour matrix are identical matrices for a tree. As an example, the detour matrix of a labeled graph G, corresponding to the carbon skeleton of spiropentane, is given in Figure 1.



$$\Delta = \begin{bmatrix} 0 & 2 & 2 & 4 & 4 \\ 2 & 0 & 2 & 4 & 4 \\ 2 & 2 & 0 & 2 & 2 \\ 4 & 4 & 2 & 0 & 2 \\ 4 & 4 & 2 & 2 & 0 \end{bmatrix}$$

Figure 1. The detour matrix of a labeled graph G corresponding to spiropentane.

The detour matrix can be computed using the following procedure. The detour matrix can be defined as follows:

$$\Delta = \sum_{l=0}^{l_{max}} \boldsymbol{B}_l \qquad (1)$$

where l_{max} is the distance of the longest possible path in a graph G, while $\boldsymbol{B}_l$ is an auxiliary matrix defined as:

$$\boldsymbol{B}_l = \begin{cases} 0 & \text{if there is a path between vertices } i \text{ and } j \text{ of length } \leq l \\ 1 & \text{otherwise} \end{cases} \qquad (2)$$

This procedure is related to Hosoya's approach to the computation of the distance matrix from the adjacency matrix of a graph.[10] The computation of the detour matrix using the above procedure is fairly simple.

The detour matrix for a complete graph has a simple form, *i.e.*, all off-diagonal elements are equal to the degree of a vertex, while the diagonal elements are, of course, equal to zero.

The detour polynomial

The characteristic polynomial $\pi(\mathrm{G}, x)$ of the detour matrix of a graph G is defined as:

$$\pi(\mathrm{G}; x) = \det |x \boldsymbol{I} - \Delta| \tag{3}$$

where $\boldsymbol{I}$ is the $N \times N$ unit matrix. We will call this polynomial the detour polynomial.

The coefficient form of the detour polynomial is given by:

$$\pi(\mathrm{G}; x) = x^N - \sum_{n=1}^{N} c_n \, x^{N-n} \tag{4}$$

or

$$\pi(\mathrm{G}; x) = x^N - c_1 \, x^{N-1} - \ldots - c_{N-1} \, x - c_N \tag{5}$$

We computed the coefficients of the detour polynomial by means of the modified Le Verrier-Faddeev-Frame (LVFF) method.[11–18] The modified LVFF method works as follows:

$$c_n = (1/n) \sum_{n=1}^{N} (\Delta_n)_{ii} \tag{6}$$

$$(\Delta_n)_{ii} = (\Delta)_{ii} \, (\boldsymbol{B}_n)_{ii} \tag{7}$$

$$(\boldsymbol{B}_n)_{ii} = (\Delta_n)_{ii} - (c_n \, \boldsymbol{I})_{ii} \tag{8}$$

$$(\boldsymbol{B}_N)_{ii} = (\Delta_N)_{ii} - (c_N \, \boldsymbol{I})_{ii} = 0 \tag{9}$$

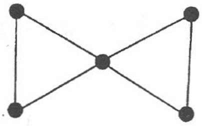
The procedure starts with the diagonalization of the detour matrix by means of the Householder-QL method[19,20] and, then, the LVFF method is carried out with Δ_n and $\boldsymbol{B}_n$ matrices in the diagonal form. We give in Table I the computation of the detour polynomial for a graph G already used in Figure 1.

In Figure 2, a number of a simple cyclic graphs are depicted. The corresponding detour polynomials are listed in Table II.

From Table II we learn that there are nonisomorphic graphs that may posses the same detour polynomial, such as the pair of graphs labeled 18 and 20 in Figure 2. This observation indicates that the detour polynomials are not more discriminating than the characteristic polynomials or distance polynomials.

TABLE I

Computation of the detour polynomial of the spiropentane graph G by the modified Le Verrier-Faddeev-Frame method



G

(1) The detour spectrum of G: {11.40312, – 1.40312, –2, –2, –6}

(2) $c_1 = \sum_i (\Delta)_{ii} = 0;\ (\Delta)_{ii} = (\Delta_1)_{ii}$

(3) $\left[(\boldsymbol{B}_1)_{ii} = (\Delta_1)_{ii} - (c_1\, \boldsymbol{I})\right]_{i=1,\ldots,5} = \{11.40312, -1.40312, -2, -2, -6\}$

$\left[(\Delta_2)_{ii} = (\Delta)_{ii}\, (\boldsymbol{B}_1)_{ii}\right]_{i=1,\ldots,5} = \{130.03114, 1.96875, 4, 4, 36\}$

$c_2 = (1/2) \sum_i (\Delta_2)_{ii} = 88$

(4) $\left[(\boldsymbol{B}_2)_{ii} = (\Delta_2)_{ii} - (c_2\, \boldsymbol{I})\right]_{i=1,\ldots,5} = \{42.03114, -86.03125, -84, -84, -52\}$

$\left[(\Delta_3)_{ii} = (\Delta)_{ii}\, (\boldsymbol{B}_2)_{ii}\right]_{i=1,\ldots,5} = \{479.28613, 120.71217, 168, 168, 312\}$

$c_3 = (1/3) \sum_i (\Delta_3)_{ii} = 416$

(5) $\left[(\boldsymbol{B}_3)_{ii} = (\Delta_3)_{ii} - (c_3\, \boldsymbol{I})\right]_{i=1,\ldots,5} = \{63.28613, -295.28783, -248, -248, -104\}$

$\left[(\Delta_4)_{ii} = (\Delta)_{ii}\, (\boldsymbol{B}_3)_{ii}\right]_{i=1,\ldots,5} = \{721.65933, 414.32426, 496, 496, 624\}$

$c_4 = (1/4) \sum_i (\Delta_4)_{ii} = 688$

(6) $\left[(\boldsymbol{B}_4)_{ii} = (\Delta_4)_{ii} - (c_4\, \boldsymbol{I})\right]_{i=1,\ldots,5} = \{33.65933, -273.67574, -192, -192, -64\}$

$\left[(\Delta_5)_{ii} = (\Delta)_{ii}\, (\boldsymbol{B}_4)_{ii}\right]_{i=1,\ldots,5} = \{384, 384, 384, 384, 384\}$

$c_5 = (1/5) \sum_i (\Delta_5)_{ii} = 384$

(7) $\left[(\boldsymbol{B}_5)_{ii} = (\Delta_5)_{ii} - (c_5\, \boldsymbol{I})\right]_{i=1,\ldots,5} = \{0, 0, 0, 0, 0\}$

(8) The detour polynomial of G

$p(\mathrm{G},x) = x^6 - 88\, x^4 - 416\, x^3 - 688\, x^2 - 384\, x$

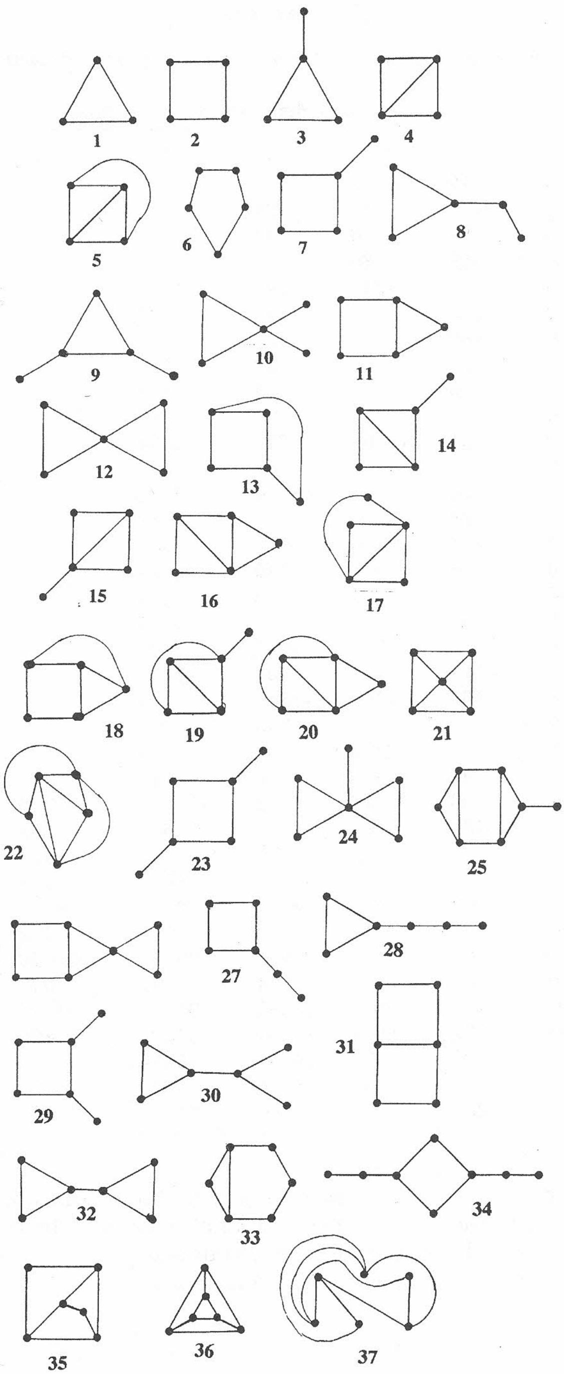


Figure 2. A selection of simple cyclic graphs.

TABLE II

Detour polynomials for a selection of simple cyclic graphs depicted in Figure 2

Cyclic graph	Coefficients of the polynomial							
	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8
1	1	0	–12	–16					
2	1	0	–44	–144	–138				
3	1	0	–31	–76	–44				
4	1	0	–49	–180	–180				
5	1	0	–54	–216	–243				
6	1	0	–125	–840	–2035	–1694			
7	1	0	–86	–412	–656	–320			
8	1	0	–68	–256	–312	–112			
9	1	0	–66	–256	–304	–112			
10	1	0	–54	–212	–280	–112			
11	1	0	–139	–1008	–2679	–2464			
12	1	0	–88	–416	–688	–384			
13	1	0	–106	–668	–1536	–1216			
14	1	0	–98	–508	–862	–444			
15	1	0	–86	–426	–699	–336			
16	1	0	–146	–1096	–3040	–2944			
17	1	0	–106	–668	–1536	–1216			
18	1	0	–153	–1184	–3408	–3456			
19	1	0	–103	–576	–1080	–594			
20	1	0	–153	–1184	–3408	–3456			
21	1	0	–160	–1280	–3840	–4096			
22	1	0	–160	–1280	–3840	–4096			
23	1	0	–144	–984	–2368	–2304	–768		
24	1	0	–97	–608	–1508	–640			
25	1	0	–506	–7348	–43972	–126272	–165328	–75840	
26	1	0	–432	–5256	–26237	–64600	–77268	–35632	
27	1	0	–157	–1012	–2404	–2368	–768		
28	1	0	–132	–704	–1348	–1040	–272		
29	1	0	–153	–1000	–2384	–2304	–768		
30	1	0	–109	–584	–1176	–992	–272		
31	1	0	–305	–3536	–16848	–36992	–30720		
32	1	0	–161	–1032	–2504	–2592	–912		
33	1	0	–298	–3368	–15396	–31744	–24144		
34	1	0	–372	–4176	–17984	–37600	–40128	–20736	–4096
35	1	0	–321	–3856	–19296	–45312	–41216		
36	1	0	–375	–5000	–28125	–75000	–78125		
37	1	0	–273	–2960	–13000	–25792	–18960		

The coefficients of the detour polynomial exhibit regularities similar to those that the coefficients of the distance polynomial also posses. The first two coefficients of the detour polynomial are, of course, equal to one and zero, respectively. The c_1-coefficient is equal to zero because of the relationship:

$$c_1 = \sum_{i=1}^{N} x_i = \mathrm{tr}\,\Delta = 0 \qquad (10)$$

The third coefficient (c_2) of the detour polynomial is equal to the half-sum of the squares of the matrix elements:

$$c_2 = (1/2) \sum_i \sum_j (\Delta^2)_{ij} \tag{11}$$

The last coefficient (c_N) of the detour polynomial is, as it is usual for all types of characteristic polynomials, given in terms of the determinant of the corresponding matrix:

TABLE III

Detour spectra for a selection of simple cyclic graphs given in Figure 2

Cyclic graph	Detour spectrum							
	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
1	4	–2	–2					
2	8	–2	–2	–4				
3	6.6	–0.9	–2	–3.7				
4	8.5	–2	–3	–3.5				
5	9	–3	–3	–3				
6	14	–2.4	–2.4	–4.6	–4.6			
7	11	–0.9	–2	–2.8	–5.6			
8	9.9	–0.6	–1.6	–2	–5.6			
9	9.8	–0.8	–1.1	–2.7	–5.2			
10	9.0	–0.7	–2	–2	–4.3			
11	14.8	–2.4	–3.4	–4.4	–4.6			
12	11.4	–1.4	–2	–2	–6			
13	12.9	–2	–2.9	–4	–4			
14	12.1	–1	–2	–3.3	–5.8			
15	11.4	–0.9	–1.9	–3.4	–5.2			
16	15.2	–2.6	–4	–4	–4.6			
17	12.9	–2	–2.9	–4	–4			
18	15.6	–3	–4	–4	–4.6			
19	12.5	–1	–3	–3	–5.6			
20	15.6	–3	–4	–4	–4.6			
21	16	–4	–4	–4	–4			
22	16	–4	–4	–4	–4			
23	14.9	–0.8	–1.1	–2	–5.2	–5.8		
24	12.5	–0.9	–2	–2	–3.6	–4		
25	28.7	–1	–2	–4	–5.5	–6	–10.1	
26	26.0	–1.4	–2	–2.5	–3.6	–4.7	–11.8	
27	15.3	–0.6	–1.6	–2	–3.1	–0.8		
28	13.8	–0.6	–0.9	–2	–2.4	–7.9		
29	15.2	–0.8	–1	–2.6	–3.2	–7.6		
30	12.7	–0.5	–1.5	–2	–2	–6.7		
31	22.4	–2.4	–4	–4	–5.4	–6.6		
32	15.5	–0.7	–2	–2	–2.5	–8.3		
33	22.0	–2	–3.1	–4.7	–6	–6.2		
34	24.1	–0.6	–0.7	–1.3	–2	–2.3	–7.1	–10.1
35	23	–4	–4	–4	–4	–7		
36	25	–5	–5	–5	–5	–5		
37	21.1	–2	–2.9	–5	–5.2	–6		

$$c_N = -\det|\Delta| \tag{12}$$

The detour polynomial of a complete graph K_N with N vertices can be given in a closed form:

$$\pi(K_N\,;x) = (x + D)^{N-1}\,(x - D^{N-2}) \tag{13}$$

where D is the degree of a vertex.

The spectrum of the detour matrix

The spectrum of the detour matrix will be called for short the detour spectrum. The detour spectra of cyclic graphs depicted in Figure 2 are given in Table III.

The detour spectrum is made up of one positive and N–1 negative elements. This particular distribution of elements of the detour spectrum is a result of the structure of the detour polynomial, that is, all coefficients, but the first coefficient, have a negative sign. The sum of elements of the detour spectrum is, of course, equal to zero. Note that the sum of squares of the elements in the detour spectrum is equal to the trace of Δ^2.

TABLE IV

The Wiener index W and the Wiener-like index ω for simple cyclic graphs from Figure 2

Cyclic graph	W	ω	Cyclic graph	W	ω
1	3	6	**20**	12	39
2	8	16	**21**	12	40
3	8	13	**22**	12	40
4	7	17	**23**	28	44
5	6	18	**24**	23	37
6	15	35	**25**	38	100
7	16	28	**26**	37	90
8	17	24	**27**	29	45
9	16	24	**28**	31	40
10	15	22	**29**	27	45
11	14	37	**30**	28	37
12	14	28	**31**	25	67
13	14	32	**32**	27	45
14	15	30	**33**	24	66
15	14	28	**34**	70	94
16	13	38	**35**	23	69
17	13	32	**36**	21	75
18	13	39	**37**	23	63
19	13	31			

The Wiener-like index ω

The Wiener-like index ω is defined in the same way as the Wiener number W,[21] that is, as the half sum of the elements of the detour matrix Δ:

$$\omega = (1/2) \sum_i \sum_j (\Delta)_{ij} \tag{13}$$

In Table IV, we give the Wiener index W and the Wiener-like index ω for graphs given in Figure 2.

Index ω for the complete graph K_N with N vertices and M edges is given by:

$$w = N\,(N-1) = M\,D \tag{14}$$

where $D = N - 1$ for complete graphs. In the case of the Wiener index, the expression for computing W for complete graphs is simpler, that is:

$$W = M \tag{15}$$

It is interesting to note that W and ω are not particularly intercorrelated quantities. The linear correlation W *vs.* ω ($\omega = a\ W + b$) for 37 graphs from Figure 2 was the poorest ($r = 0.79$) and the exponential relationship ($\omega = a\ W^b$) produced the best correlation coeficient ($r = 0.86$), but still far from the values for strongly intercorrelated quantities. The potential of the Wiener-like index ω is still unknown and is presently under investigation.

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SAŽETAK

O matrici zaobilaznih udaljenosti

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Razmatrana je matrica zaobilaznih udaljenosti grafa i njezine invarijante (polinom, spektar i numerički indeks nalik Wienerovu broju). Prikazane su metoda računanja matrice zaobilaznih udaljenosti i njezinih invarijanti. Dane su također i neke usporedbe s matricom udaljenosti grafa.