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The Detour Matrix and the Detour Index of Weighted Graphs*

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The detour matrix of a weighted graph and its invariants (the detour polynomial, the detour spectrum, the detour index) are discussed. A novel method for computing the detour matrix of (weighted) graphs is proposed.

The detour matrix was recently discussed in this journal.[1] This matrix was introduced into the mathematical literature in 1990 by Buckley and Harary in their book on the distance matrix.[2] The detour matrix has been introduced into the chemical literature in 1994 under the name the maximum path matrix of a molecular graph by Ivanciuc and Balaban.[3] The corresponding Wiener-like index, called the detour index by Lukovits,[4] was introduced by Ivanciuc and Balaban[3] as the half-sum of the maximum path sums. The detour index was also discussed by us[1] and by Lukovits.[4,5] Lukovits was also first to use this index in the structure-property modeling and

* Dedicated to the memory of Professor Stanko Borčić (Shangai, March 1, 1931 – Zagreb, December 21, 1994), one of the most prominent Croatian chemists of our times.

has found[4] that the detour index combined with the Wiener index is quite efficient in QSPR[6] studies if a series of molecules considered consists of acyclic and cycle-containing molecules. Lukovits also delivered a very stimulating talk on this work at the Rugjer Bošković Institute in Zagreb on February 29, 1996.

It should be noted that most graph-theoretical indices proposed to date are not efficient when both acyclic and cycle-containing molecules are considered in the structure-property study; the connectivity index[7] and in some cases the Wiener index[8] are exceptions.[9,10] However, the above finding warrants further studies on the detour matrix and the detour index. In this paper we report the extension of the detour matrix to weighted graphs representing heterosystems.[11(a)]

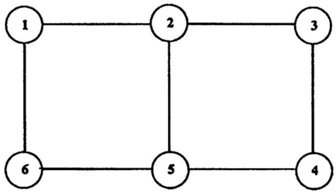
The detour matrix $\Delta = \Delta(\mathrm{G})$ of a labeled connected graph G is a real symmetric $N \times N$ matrix whose (i,j)-entry is the length of the longest path[11(b)] from vertex i to vertex j. This definition is the »opposite« of the definition of the traditional graph-theoretical distance matrix, whose off-diagonal entries are the lengths of the shortest paths between the vertices in G.[11(c)–13] It is obvious from their definitions that the detour matrix and the distance matrix are identical for trees.

The construction of the detour matrix for larger graphs (molecules) is not a trivial task. Lukovits[5] pointed out quite correctly that the usefulness of the detour index is diminished by the fact that to date no method (but inspection) is available to compute this index. However, we have succeeded in finding a moderately efficient approach to compute the detour matrix and consequently the detour index of graphs.[14] This procedure is later described and exemplified in the text.

The detour index ω is defined in the same way as the Wiener index,[15,16] that is, the detour index is equal to the half-sum of the elements of the detour matrix Δ:[3]

$$\omega = \frac{1}{2} \sum_i \sum_j (\Delta)_{ij} \qquad (1)$$

The Wiener index W and the detour index ω are, of course, identical for acyclic structures. For polycyclic structures, W and ω are not particularly intercorrelated indices. For example, the linear correlation between W and ω ($\omega = aW + b$) for a set of 37 diverse polycyclic graphs has a modest correlation coefficient ($r = 0.79$), while the exponential relationship between W and ω ($\omega = aW^b$) produced only a little better correlation between them ($r = 0.86$).[1] In Figure 1 we give the distance and detour matrices for a bicyclic graph G and the corresponding Wiener and detour indices.



G

$$
\boldsymbol{D} = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix} \qquad \Delta = \begin{bmatrix} 0 & 5 & 4 & 5 & 4 & 5 \\ 5 & 0 & 5 & 4 & 3 & 4 \\ 4 & 5 & 0 & 5 & 4 & 5 \\ 5 & 4 & 5 & 0 & 5 & 4 \\ 4 & 3 & 4 & 5 & 0 & 5 \\ 5 & 4 & 5 & 4 & 5 & 0 \end{bmatrix}
$$

$$W = 25 \qquad \omega = 67$$

Figure 1. The distance matrix $\boldsymbol{D}$ and the detour matrix Δ of a labeled bicyclic graph G and the corresponding Wiener index and the detour index.

In the case of of weighted graphs $G_{w,}$ the detour matrix entries $(\Delta_w)_{ij} = [\Delta(G_w)]_{ij}$ are defined as:

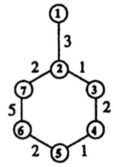
$$
(\Delta_w)_{ij} = \begin{cases} w_{ij} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \tag{2}
$$

where w_{ij} is the maximum sum of edge-weights along the path between the vertices i and j, which is not necessarily the longest possible path between these two vertices in G_w as it would be in terms of just unweighted edges. Hence, in the case of the weighted detour matrix, the entry $(\Delta_w)_{ij}$ is the maximum path-weight between the vertices i and j in G_w. The distance and detour matrices for an edge-weighted graph G_w and the corresponding Wiener and detour indices are given in Figure 2.

Our method for computing the detour matrix of a polycyclic graph G, and consequently the detour index, is based on considering the distance matrices of the whole set of spanning trees obtained from G by deletion of the appropriate edges. The procedure consist of the following steps:

(i) Labeling of a graph G under the consideration.

(ii) Generation of labeled spanning trees from G and the construction of their distance matrices.



G_w

$$D_w = \begin{bmatrix} 0 & 3 & 4 & 6 & 7 & 9 & 5 \\ 3 & 0 & 1 & 3 & 4 & 6 & 2 \\ 4 & 1 & 0 & 2 & 3 & 5 & 3 \\ 6 & 3 & 1 & 0 & 1 & 3 & 5 \\ 7 & 4 & 3 & 1 & 0 & 2 & 6 \\ 9 & 6 & 5 & 3 & 2 & 0 & 5 \\ 5 & 2 & 3 & 5 & 6 & 5 & 0 \end{bmatrix} \qquad \Delta_w = \begin{bmatrix} 0 & 3 & 15 & 13 & 12 & 10 & 14 \\ 3 & 0 & 12 & 10 & 9 & 7 & 11 \\ 15 & 12 & 0 & 11 & 10 & 8 & 10 \\ 13 & 10 & 11 & 0 & 12 & 10 & 8 \\ 12 & 9 & 10 & 12 & 0 & 11 & 7 \\ 10 & 7 & 8 & 10 & 11 & 0 & 8 \\ 14 & 11 & 10 & 8 & 7 & 8 & 0 \end{bmatrix}$$

$W = 85$ $\qquad$ $\omega = 211$

Figure 2. The distance matrix $\boldsymbol{D}_w$ and the detour matrix Δ_w of a labeled weighted graph G_w and the corresponding Wiener index and the detour index.

(iii) Setting up the detour matrix of G by matching the distance matrices of spanning trees and picking up for each element of the detour matrix only that distance matrix element which possesses the highest numerical value.

A computer program based on this procedure will appear elsewhere. This procedure for a simple unweighted bicyclic graph G (already shown in Figure 1) and weighted bicyclic graph G_w is illustrated in Figures 3 and 4.

The characteristic polynomial $\pi(G_w; x)$ of the detour matrix, called the detour polynomial,[1] of a weighted graph G_w is defined as:

$$\pi(G_w; x) = \det \left| x\boldsymbol{I} - \Delta_w \right| \tag{3}$$

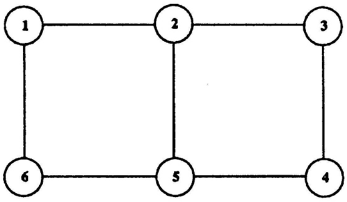
where $\boldsymbol{I}$ is the $N \times N$ unit matrix. The coefficient form of the detour polynomial is given by:

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

or

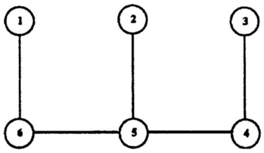
$$\pi(G_w; x) = x^N - c_1 \, x^{N-1} - \ldots - c_{N-1} x - c_N \tag{5}$$

(1) Labeled bicyclic graph G



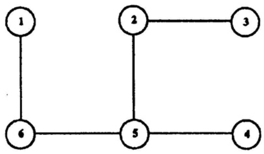
G

(2) Labeled spanning trees of G



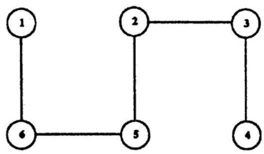
G_1

$$D(G_1) = \begin{bmatrix} 0 & 3 & 4 & 3 & 2 & 1 \\ 3 & 0 & 3 & 2 & 1 & 2 \\ 4 & 3 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$



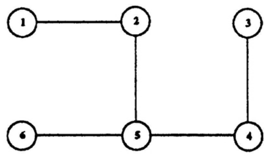
G_2

$$D(G_2) = \begin{bmatrix} 0 & 3 & 4 & 3 & 2 & 1 \\ 3 & 0 & 1 & 2 & 1 & 2 \\ 4 & 1 & 0 & 3 & 2 & 3 \\ 3 & 2 & 3 & 0 & 1 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$



G_3

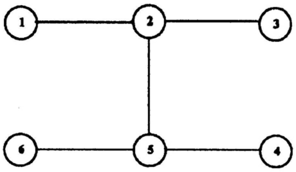
$$D(G_3) = \begin{bmatrix} 0 & 3 & 4 & 5 & 2 & 1 \\ 3 & 0 & 1 & 2 & 1 & 2 \\ 4 & 1 & 0 & 1 & 2 & 3 \\ 5 & 2 & 1 & 0 & 3 & 4 \\ 2 & 1 & 2 & 3 & 0 & 1 \\ 1 & 2 & 3 & 4 & 1 & 0 \end{bmatrix}$$



G_4

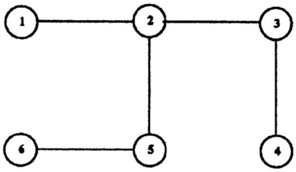
$$D(G_4) = \begin{bmatrix} 0 & 1 & 4 & 3 & 2 & 3 \\ 1 & 0 & 3 & 2 & 1 & 2 \\ 4 & 3 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 \\ 3 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$

Figure 3. The construction of the detour matrix for the simple bicyclic graph G from Figure 1.



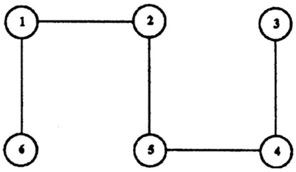
G_5

$$D(G_5) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 3 \\ 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 3 & 2 & 3 \\ 3 & 2 & 3 & 0 & 1 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 \\ 3 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$



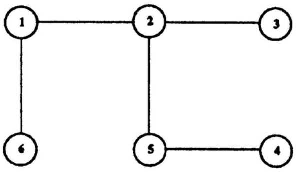
G_6

$$D(G_6) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 3 \\ 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 3 & 4 \\ 2 & 1 & 2 & 3 & 0 & 1 \\ 3 & 2 & 3 & 4 & 1 & 0 \end{bmatrix}$$



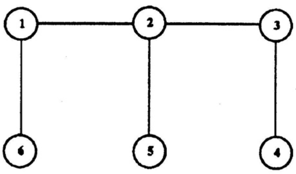
G_7

$$D(G_7) = \begin{bmatrix} 0 & 1 & 4 & 3 & 2 & 1 \\ 1 & 0 & 3 & 2 & 1 & 2 \\ 4 & 3 & 0 & 1 & 2 & 5 \\ 3 & 2 & 1 & 0 & 1 & 4 \\ 2 & 1 & 2 & 1 & 0 & 3 \\ 1 & 2 & 5 & 4 & 3 & 0 \end{bmatrix}$$



G_8

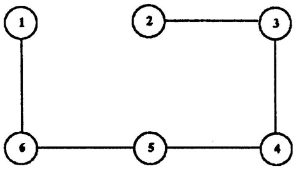
$$D(G_8) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 3 & 2 & 3 \\ 3 & 2 & 3 & 0 & 1 & 4 \\ 2 & 1 & 2 & 1 & 0 & 3 \\ 1 & 2 & 3 & 4 & 3 & 0 \end{bmatrix}$$



G_9

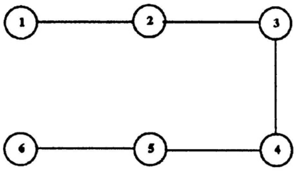
$$D(G_9) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 3 & 4 \\ 2 & 1 & 2 & 3 & 0 & 3 \\ 1 & 2 & 3 & 4 & 3 & 0 \end{bmatrix}$$

Figure 3, continued.



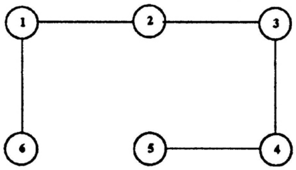
G_{10}

$$D(G_{10}) = \begin{bmatrix} 0 & 5 & 4 & 3 & 2 & 1 \\ 5 & 0 & 1 & 2 & 3 & 4 \\ 4 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 4 & 3 & 2 & 1 & 0 \end{bmatrix}$$



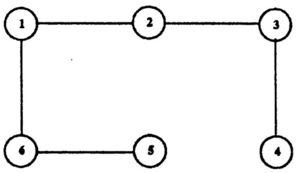
G_{11}

$$D(G_{11}) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 2 & 3 & 4 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 4 & 3 & 2 & 1 & 0 & 1 \\ 5 & 4 & 3 & 2 & 1 & 0 \end{bmatrix}$$



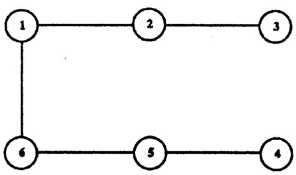
G_{12}

$$D(G_{12}) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 4 \\ 4 & 3 & 2 & 1 & 0 & 5 \\ 1 & 2 & 3 & 4 & 5 & 0 \end{bmatrix}$$



G_{13}

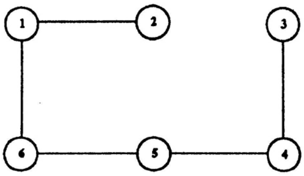
$$D(G_{13}) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 4 & 3 \\ 3 & 2 & 1 & 0 & 5 & 4 \\ 2 & 3 & 4 & 5 & 0 & 1 \\ 1 & 2 & 3 & 4 & 1 & 0 \end{bmatrix}$$



G_{14}

$$D(G_{14}) = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 4 & 3 & 2 \\ 2 & 1 & 0 & 5 & 4 & 3 \\ 3 & 4 & 5 & 0 & 1 & 2 \\ 2 & 3 & 4 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$

Figure 3, continued.



G_{15}

$$D(G_{15}) = \begin{bmatrix} 0 & 1 & 4 & 3 & 2 & 1 \\ 1 & 0 & 5 & 4 & 3 & 2 \\ 4 & 5 & 0 & 1 & 2 & 3 \\ 3 & 4 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$

(3) Detour matrix of G

$$\Delta(G) = \begin{bmatrix} 0 & 5 & 4 & 5 & 4 & 5 \\ 5 & 0 & 5 & 4 & 3 & 4 \\ 4 & 5 & 0 & 5 & 4 & 5 \\ 5 & 4 & 5 & 0 & 5 & 4 \\ 4 & 3 & 4 & 5 & 0 & 5 \\ 5 & 4 & 5 & 4 & 5 & 0 \end{bmatrix}$$

Figure 3, continued from pp. 1581–1583.

The coefficients c_n of the detour polynomial of weighted graphs can be computed using the modified Le Verrier-Faddeev-Frame (LVFF) method.[1,11(d),13, 17–20] This can be done by using the detour matrix Δ and the auxiliary matrices $\boldsymbol{C}_n$ (n = 1, 2, ..., N):

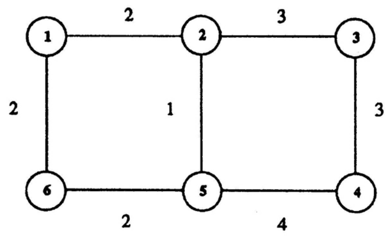
$$c_n = \frac{1}{n} \sum_{n=1}^{N} (\Delta_n)_{ii} \tag{6}$$

$$(\Delta_n)_{ii} = (\Delta)_{ii}\, (\boldsymbol{C}_{\mathrm{n}})_{ii} \tag{7}$$

$$(\boldsymbol{C}_{\mathrm{n}})_{ii} = (\Delta_n)_{ii} - (c_n\, \boldsymbol{I})_{ii} \tag{9}$$

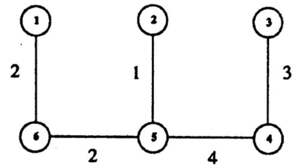
$$(\boldsymbol{C}_N)_{ii} = (\Delta_N)_{ii} - (c_N\, \boldsymbol{I})_{ii} = \boldsymbol{0} \tag{10}$$

The procedure starts with the diagonalization of the detour matrix by means of the Householder-QL method[21] and, then, the LVFF method is carried out with Δ_n and $\boldsymbol{C}_n$ matrices in the diagonal form. The procedure ends when the auxilliary matrix $\boldsymbol{C}_{\mathrm{n}}$ becomes the null-matrix. The computation of the detour polynomial for a weighted graph G_w on five vertices is shown in Table I.



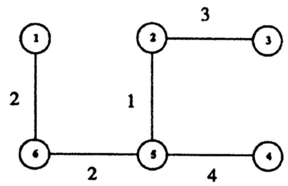
G_w

(2) Labeled weighted spanning trees of G_w



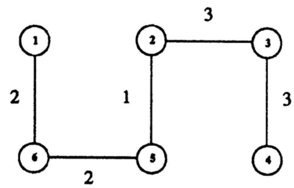
G_1

$$D(G_1) = \begin{bmatrix} 0 & 5 & 11 & 8 & 4 & 2 \\ 5 & 0 & 8 & 5 & 1 & 3 \\ 11 & 8 & 0 & 3 & 7 & 9 \\ 8 & 5 & 3 & 0 & 4 & 6 \\ 4 & 1 & 7 & 4 & 0 & 2 \\ 2 & 3 & 9 & 6 & 2 & 0 \end{bmatrix}$$



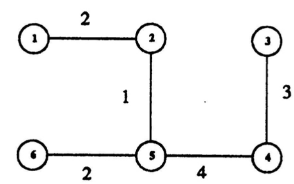
G_2

$$D(G_2) = \begin{bmatrix} 0 & 5 & 8 & 8 & 4 & 2 \\ 5 & 0 & 3 & 5 & 1 & 3 \\ 8 & 8 & 0 & 8 & 4 & 6 \\ 8 & 5 & 8 & 0 & 4 & 6 \\ 4 & 1 & 4 & 4 & 0 & 2 \\ 2 & 3 & 6 & 6 & 2 & 0 \end{bmatrix}$$



G_3

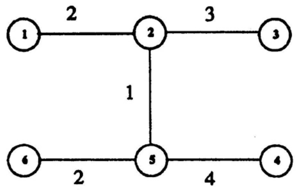
$$D(G_3) = \begin{bmatrix} 0 & 5 & 8 & 11 & 4 & 2 \\ 5 & 0 & 3 & 6 & 1 & 3 \\ 8 & 3 & 0 & 3 & 4 & 6 \\ 11 & 6 & 3 & 0 & 7 & 9 \\ 4 & 1 & 4 & 7 & 0 & 2 \\ 2 & 3 & 6 & 9 & 2 & 0 \end{bmatrix}$$



G_4

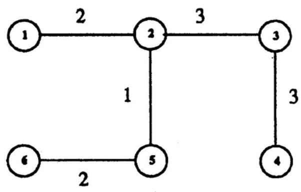
$$D(G_4) = \begin{bmatrix} 0 & 5 & 8 & 11 & 4 & 2 \\ 5 & 0 & 3 & 6 & 1 & 3 \\ 8 & 3 & 0 & 3 & 4 & 6 \\ 11 & 6 & 3 & 0 & 7 & 9 \\ 4 & 1 & 4 & 7 & 0 & 2 \\ 2 & 3 & 6 & 9 & 2 & 0 \end{bmatrix}$$

Figure 4. The construction of the detour matrix for the simple weighted bicyclic graph G_w.



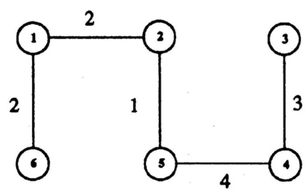
G_5

$$D(G_5) = \begin{bmatrix} 0 & 2 & 5 & 7 & 3 & 5 \\ 2 & 0 & 3 & 5 & 1 & 3 \\ 5 & 3 & 0 & 8 & 4 & 6 \\ 7 & 5 & 8 & 0 & 4 & 6 \\ 3 & 1 & 4 & 4 & 0 & 2 \\ 5 & 3 & 6 & 6 & 2 & 0 \end{bmatrix}$$



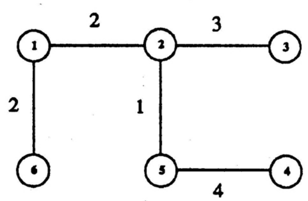
G_6

$$D(G_6) = \begin{bmatrix} 0 & 2 & 5 & 8 & 3 & 5 \\ 2 & 0 & 3 & 6 & 1 & 3 \\ 5 & 3 & 0 & 3 & 4 & 6 \\ 8 & 6 & 3 & 0 & 7 & 9 \\ 3 & 1 & 4 & 7 & 0 & 2 \\ 5 & 3 & 6 & 9 & 2 & 0 \end{bmatrix}$$



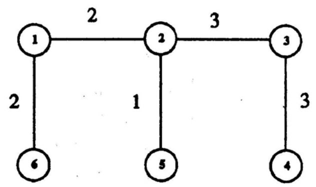
G_7

$$D(G_7) = \begin{bmatrix} 0 & 2 & 10 & 7 & 3 & 2 \\ 2 & 0 & 8 & 5 & 1 & 4 \\ 10 & 8 & 0 & 3 & 7 & 12 \\ 7 & 5 & 3 & 0 & 4 & 9 \\ 3 & 1 & 7 & 4 & 0 & 5 \\ 2 & 4 & 12 & 9 & 5 & 0 \end{bmatrix}$$



G_8

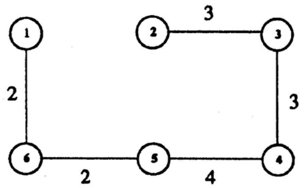
$$D(G_8) = \begin{bmatrix} 0 & 2 & 5 & 7 & 3 & 2 \\ 2 & 0 & 3 & 5 & 1 & 4 \\ 5 & 3 & 0 & 8 & 4 & 7 \\ 7 & 5 & 8 & 0 & 4 & 9 \\ 3 & 1 & 4 & 4 & 0 & 5 \\ 2 & 4 & 7 & 9 & 5 & 0 \end{bmatrix}$$



G_9

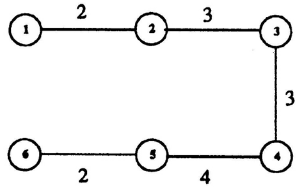
$$D(G_9) = \begin{bmatrix} 0 & 2 & 5 & 8 & 3 & 2 \\ 2 & 0 & 3 & 6 & 1 & 4 \\ 5 & 3 & 0 & 3 & 4 & 7 \\ 8 & 6 & 3 & 0 & 7 & 10 \\ 3 & 1 & 4 & 7 & 0 & 5 \\ 2 & 4 & 7 & 10 & 5 & 0 \end{bmatrix}$$

Figure 4, continued.



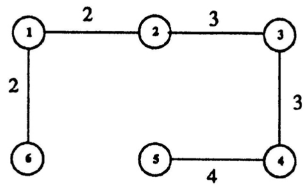
G_{10}

$$D(G_{10}) = \begin{bmatrix} 0 & 14 & 11 & 8 & 4 & 2 \\ 14 & 0 & 3 & 6 & 10 & 12 \\ 11 & 3 & 0 & 3 & 7 & 9 \\ 8 & 6 & 3 & 0 & 4 & 6 \\ 4 & 10 & 7 & 4 & 0 & 2 \\ 2 & 12 & 9 & 6 & 2 & 0 \end{bmatrix}$$



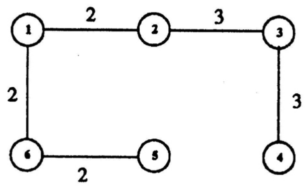
G_{11}

$$D(G_{11}) = \begin{bmatrix} 0 & 2 & 5 & 8 & 12 & 14 \\ 2 & 0 & 3 & 6 & 10 & 12 \\ 5 & 3 & 0 & 3 & 7 & 9 \\ 8 & 6 & 3 & 0 & 4 & 6 \\ 4 & 10 & 7 & 4 & 0 & 2 \\ 2 & 12 & 9 & 6 & 2 & 0 \end{bmatrix}$$



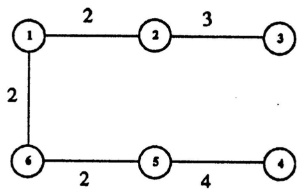
G_{12}

$$D(G_{12}) = \begin{bmatrix} 0 & 2 & 5 & 8 & 12 & 2 \\ 2 & 0 & 3 & 6 & 10 & 4 \\ 5 & 3 & 0 & 3 & 7 & 7 \\ 8 & 6 & 3 & 0 & 4 & 10 \\ 12 & 10 & 7 & 4 & 0 & 14 \\ 2 & 4 & 7 & 10 & 14 & 0 \end{bmatrix}$$



G_{13}

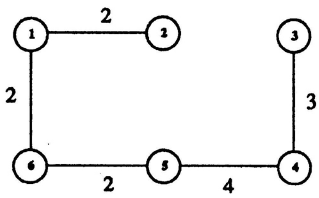
$$D(G_{13}) = \begin{bmatrix} 0 & 2 & 5 & 8 & 4 & 2 \\ 2 & 0 & 3 & 6 & 6 & 4 \\ 5 & 3 & 0 & 3 & 9 & 7 \\ 8 & 6 & 3 & 0 & 12 & 10 \\ 4 & 6 & 9 & 12 & 0 & 2 \\ 2 & 4 & 7 & 10 & 2 & 0 \end{bmatrix}$$



G_{14}

$$D(G_{14}) = \begin{bmatrix} 0 & 2 & 5 & 8 & 4 & 2 \\ 2 & 0 & 3 & 10 & 6 & 4 \\ 5 & 3 & 0 & 13 & 9 & 7 \\ 8 & 10 & 13 & 0 & 4 & 6 \\ 4 & 6 & 9 & 4 & 0 & 2 \\ 2 & 4 & 7 & 6 & 2 & 0 \end{bmatrix}$$

Figure 4, continued.



G_{15}

$$D(G_{15}) = \begin{bmatrix} 0 & 2 & 11 & 8 & 4 & 2 \\ 2 & 0 & 13 & 10 & 6 & 4 \\ 11 & 13 & 0 & 3 & 7 & 9 \\ 8 & 10 & 3 & 0 & 4 & 6 \\ 4 & 6 & 7 & 4 & 0 & 2 \\ 2 & 4 & 9 & 6 & 2 & 0 \end{bmatrix}$$

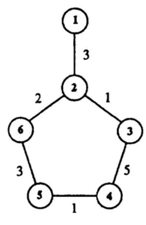
(3) Detour matrix of the weighted bicyclic graph G_w

$$\Delta(G_w) = \begin{bmatrix} 0 & 14 & 13 & 10 & 12 & 14 \\ 14 & 0 & 13 & 10 & 10 & 12 \\ 13 & 13 & 0 & 13 & 9 & 12 \\ 10 & 10 & 13 & 0 & 12 & 10 \\ 12 & 10 & 9 & 12 & 0 & 14 \\ 14 & 12 & 12 & 10 & 14 & 0 \end{bmatrix}$$

Figure 4, continued from pp. 1585–1587.

TABLE I

Computation of the detour polynomial of a weighted graph G_w on five vertices using the modified Le Verrier-Faddeev-Frame method



G_w

(1) The detour spectrum of G_w

{4.472902898666935e+01, –1.891336860675328e+01, –1.137548047084902e+01, –9.019959525687815e+00, –3.746409753799866e+00, –1.673810629579382e+00}

TABLE I, continued.

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

(3) $[(\boldsymbol{C}_1)_{ii} = (\Delta)_{ii} - (c_1\boldsymbol{I})]_{i=1,\dots,6} =$

{4.472902898666935e+01, –1.891336860675328e+01, –1.137548047084902e+01, –9.019959525687815e+00, –3.746409753799866e+00, –1.673810629579382e+00}

$[(\Delta_2)_{ii} = (\Delta)_{ii} \cdot (\boldsymbol{C}_1)_{ii}]_{i=1,\dots,6} =$

{1.403558604336678e+01, 2.801642023692891e+00, 8.135966984504609e+01, 1.294015559426670e+02, 3.577155120549204e+02, 2.000686034090305e+03}

$$c_2 = \frac{1}{2}\sum_i (\Delta_2)_{ii} = 1293$$

(4) $[(\boldsymbol{C}_2)_{ii} = (\Delta_2)_{ii} - (c_2\boldsymbol{I})]_{i=1,\dots,6} =$

{–1.278964413956632e+03, –1.290198357976306e+03, –1.211640330154954e+03, –1.163598444057332e+e3, –9.352844879450788e+02, 7.076860340903061e+02}

$[(\Delta_3)_{ii} = (\Delta)_{ii} \cdot (\boldsymbol{C}_2)_{ii}]_{i=1,\dots,6} =$

{4.791524755210062e+03, 2.159547725846602e+03, 1.092894673768871e+04, 1.323649137628450e+04, 1.768938027268379e+04, 3.165410913228638e+04}

$$c_3 = \frac{1}{3}\sum_i (\Delta_3)_{ii} = 26820$$

(5) $[(\boldsymbol{C}_3)_{ii} = (\Delta_3)_{ii} - (c_3\boldsymbol{I})]_{i=1,\dots,6} =$

{–2.202847524478994e+04, –2.466045227415340e+04, –1.589105326231130e+04, –1.358350862371552e+e4, –9.130619727316220e+03, 4.834109132286384e+03}

$[(\Delta_4)_{ii} = (\Delta)_{ii} \cdot (\boldsymbol{C}_3)_{ii}]_{i=1,\dots,6} =$

{1.545189370746849e+05, 1.433366572465972e+05, 1.726907765108247e+05, 8.252769451841983e+04, 2.162250075027603e+05, 4.127692714671288e+04}

$$c_4 = \frac{1}{4}\sum_i (\Delta_4)_{ii} = 202644$$

(6) $[(\boldsymbol{C}_4)_{ii} = (\Delta_4)_{ii} - (c_4\boldsymbol{I})]_{i=1,\dots,6} =$

{–4.812506292531502e+04, –5.930734275340284e+04, –2.995322348917524e+04, –1.201163054815800e+05, 1.358100750276040e+04, –1.613670728532870e+05}

$[(\Delta_5)_{ii} = (\Delta)_{ii} \cdot (\boldsymbol{C}_4)_{ii}]_{i=1,\dots,6} =$

{5.474457134653004e+05, 5.349498312117877e+05, 5.665163568112324e+05, 6.074652782591418e+05, 4.500048984465956e+05, 2.700979218059412e+05}

$$c_5 = \frac{1}{5}\sum_i (\Delta_5)_{ii} = 595296$$

TABLE I, continued.

(**7**) $[(\boldsymbol{C}_5)_{ii} = (\Delta_5)_{ii} - (c_5\boldsymbol{I})]_{i=1,...,6} =$

$\{-4.785028653469921e+04, -6.034616878821229e+04, -2.877964318876770e+04, 1.216927825914188e+04, -1.452911015534041e+05, -3.251980781940584e+05\}$

$[(\Delta_6)_{ii} = (\Delta)_{ii} \cdot (\boldsymbol{C}_5)_{ii}] = \{544320, 544320, 544320, 544320, 544320, 544320\}$

$$c_6 = \frac{1}{6}\sum_i (\Delta_6)_{ii} = 0$$

(**8**) The detour polynomial of G_w

$\pi(G_w; x) = x^6 - 1293\, x^4 - 26820\, x^3 - 202644\, x^2 - 595296\, x - 544320$

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SAŽETAK

Matrica zaobilaznosti i indeks zaobilaznosti vaganih grafova

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Razmatrana je matrica zaobilaznosti vaganih grafova i njezine invarijante (polinom zaobilaznosti, spektar zaobilaznosti, indeks zaobilaznosti). Predložena je nova metoda za sastavljanje matrice zaobilaznih udaljenosti.