A Novel Definition of the Wiener Index for Trees

Bojan Mohar

Department of Mathematics, The University of Ljubljana, SI-61111 Ljubljana, The Republic of Slovenia

Darko Babić and Nenad Trinajstić*

The Rugjer Bošković Institute, HR-41001 Zagreb, The Republic of Croatia

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The Wiener index for a tree is redefined in terms of eigenvalues of the corresponding Laplacian matrix.

The Wiener index[1] is one of the oldest and most widely used topological indices in the quantitative structure–property relationships (QSPR).[2,3] Originally the Wiener index was defined as the sum of the distances between any two carbon atoms in an alkane, in terms of carbon–carbon bonds, and was named the path number. Wiener[1] also suggested a simple method for the calculation of the path number: Multiply the number of carbon atoms on one side of any bond by those on the other side; W is then the sum of these products. In the initial applications, the Wiener index was employed to predict physical parameters such as boiling points, heats of formation, heats of vaporization, molar volumes, and molar refractions of alkanes by the use of simple QSPR models.[1,4–9]

In his papers, Wiener did not use the graph-theoretical language, and the application of the path number was confined to acyclic systems. The Wiener index was first defined within the framework of chemical graph theory by Hosoya,[10] in 1971, who pointed out that this index (he called it the Wiener number) can be obtained from the distance matrix $\mathbf{D} = \mathbf{D}(G)$ of a molecular graph G. This topological index, denoted by W in honor of Wiener, is a number equal to the half-sum of the elements of the distance matrix:

$$W = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{D})_{ij} \qquad (1)$$

where $(\mathbf{D})_{ij}$ are the off-diagonal elements of $\mathbf{D}$, and N is the number of vertices in G.

We offer in this paper a novel graph-theoretical definition of the Wiener index for trees, based on the Laplacian matrix. The Laplacian matrix $\mathbf{L} = \mathbf{L}(G)$ of a graph G is defined[11,12] as the following difference matrix:

$$\mathbf{L} = \mathbf{V} - \mathbf{A} \qquad (2)$$

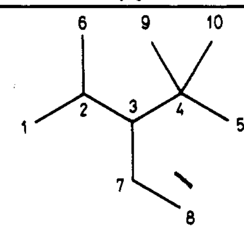
where $\mathbf{A}$ is the adjacency matrix, and $\mathbf{V}$ is the degree (valency) matrix, i.e., the diagonal matrix with entries

$$(\mathbf{V})_{ii} = D(i) \qquad (3)$$

where $D(i)$ is the degree (valency) of the vertex i in G. For example, the Laplacian matrix of a tree T, depicting the carbon skeleton of 3-ethyl-2,2,4-trimethylpentane, is given in Table I.

The matrix $\mathbf{L}$ is sometimes also called the Kirchhoff matrix[12,13] of a graph because of its role in the Matrix-Tree Theorem, which is usually attributed to Kirchhoff. Another name for this matrix is the matrix of admittance,[11,14] which originates in the theory electrical networks (admittance = conductivity). However, the name Laplacian matrix is more appropriate since $\mathbf{L}$ is just the matrix of a discrete Laplacian operator.[15]

Table I. Laplacian Matrix of Tree T Corresponding to Carbon Skeleton of 3-Ethyl-2,2,4-trimethylpentane



T

$$\mathbf{L} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 4 & -1 & 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The Laplacian matrix is real symmetric matrix. The diagonalization of the Laplacian matrix for a graph G with N vertices produces N real eigenvalues $0 = x_1 \le x_2 \le ... \le x_N$. Let a graph G be a tree, then the Wiener index of a tree T can be given in terms of its Laplacian eigenvalues as follows:

$$W = N\sum_{i=2}^{N}\frac{1}{x_i} \qquad (4)$$

This formula can be proven in the following way. x_n are zeros of the characteristic polynomial $\mu(x)$ of the Laplacian matrix:

$$\mu(x) = x^N + c_{N-1}x^{N-1} + ... + c_2x^2 + c_1x + c_0 \qquad (5)$$

Vieta's formulas relate the coefficients and zeros of $\mu(x)$ as follows:

$$c_0 = (-1)^N x_1 x_2 ... x_N = 0 \quad (\text{since } x_1 = 0) \qquad (6)$$

$$c_1 = (-1)^{N-1}[x_2x_3 ... x_N + x_1x_3 ... x_N + ... + x_1x_2 ... x_{N-1}] = (-1)^{N-1}x_2x_3 ... x_N \qquad (7)$$

$$c_2 = (-1)^{N-2}[\text{sum of all } (N-2) \text{ tuples of } \{x_1, x_2, ..., x_N\}] \qquad (8)$$

The summation factor in eq 4 can be rewritten by taking the common divisor and applying the above Vieta's relations, as

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