Hyper-Wiener Vector, Wiener Matrix Sequence, and Wiener Polynomial Sequence of a Graph

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ABSTRACT: The Wiener matrix and the hyper-Wiener number of a tree (acyclic structure) were first introduced by Randic [1]. Randic and Guo and colleagues [2, 3] further introduced the higher Wiener numbers of a tree that can be represented by a Wiener number sequence ${}^1W$, ${}^2W$, ${}^3W, \ldots$, where ${}^1W = W$ is the Wiener index, and $\sum_{k=1,2,\cdots} {}^kW = R$ is the hyper-Wiener number. Later the definition of hyper-Wiener number was extended by Klein et al. for application to any connected structure. In this study, the definition of higher Wiener numbers is extended to be applicable to any connected structure. The concepts of the Wiener vector and hyper-Wiener vector of a graph are introduced. Moreover, a matrix sequence $\mathbf{W}^{(1)}, \mathbf{W}^{(2)}, \mathbf{W}^{(3)}, \ldots$, called the Wiener matrix sequence (or distance matrix sequence), and their sum $\sum_{k=1,2,\cdots} \mathbf{W}^{(k)} = \mathbf{W}^{(H)}$, called the hyper-Wiener matrix, are introduced, where $\mathbf{W}^{(1)} = \mathbf{D}$ is the distance matrix, and the sum of the entries of upper triangle of $\mathbf{W}^{(k)}$ (resp. $\mathbf{W}^{(H)}$) is just equal to ${}^kW$ (resp. R). A Wiener polynomial sequence and a weighted hyper-Wiener polynomial of a graph are also introduced. Int J Quantum Chem 106: 1756–1761, 2006

Key words: hyper-Wiener vector; weighted Wiener polynomial; Wiener polynomial sequence; Wiener matrix sequence

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Introduction

The Wiener matrix and hyper-Wiener number of a tree T (acyclic structure) were first introduced by Randic [1]. For any two vertices i, j in T, let $\pi(i, j)$ denote the unique path in T with end vertices i, j and the length d_{ij}, let $T_{1,\pi(i,j)}$ and $T_{2,\pi(i,j)}$ denote the components of $T - E[\pi(i, j)]$ containing i and j, respectively, and let $n_{1,\pi(i,j)}$ and $n_{2,\pi(i,j)}$ denote the numbers of the vertices in $T_{1,\pi(i,j)}$ and $T_{1,\pi(i,j)}$, respectively. The Wiener matrix $\mathbf{W}$ and the hyper-Wiener number R of T can then be given by

$$\mathbf{W} = (w_{ij}), \qquad w_{ij} = n_{1,\pi(i,j)}n_{2,\pi(i,j)},$$

$$R = \sum_{i<j} w_{ij}.$$

In Refs. [2, 3], Randic and Guo and colleagues further introduced the higher Wiener numbers and some other Wiener matrix invariants of a tree T. The higher Wiener numbers can be represented by a Wiener number sequence ${}^1W$, ${}^2W$, ${}^3W$, . . . , where ${}^kW = \sum_{d_{ij}=k,i<j} w_{ij}$. It is not difficult to see that ${}^1W = W$, and $\sum_{k=1,2,\cdots} {}^kW = R$.

After the hyper-Wiener number of a tree was introduced, many publications [4–19] have appeared on the calculation and generalization of the hyper-Wiener number.

Klein et al. [4] generalized the hyper-Wiener number so as to be applicable to any connected structure. Their formula for the hyper-Wiener number R of a graph G is

$$R(G) = R = \tfrac{1}{2} \sum_{i<j} (d_{ij}^2 + d_{ij}).$$

Replacing d_{ij} by Ω_{ij} in the above formula, Klein et al. [4] give a different extension of hyper-Wiener numbers for general graphs, where Ω_{ij} denotes the resistance distance between two vertices i and j, which is just the effective electrical resistance between i and j when unit resistors are placed on each edge. Some other generalizations of the hyper-Wiener number for any graphs were given by Lukovits and colleagues [5], Li [8], Gutman [9]. The relationship between the Wiener polynomial (or Hosoya polynomial) and the hyper-Wiener number was given by Cash [19].

Note that two trees with the same hyper-Wiener number might have different Wiener number sequences, and two trees with the same Wiener number sequence might have different Wiener matrices. In other words, Wiener number sequences have higher discrimination than do hyper-Wiener numbers, and Wiener matrices have higher discrimination than do Wiener number sequences. Wiener number sequences and Wiener matrices will be useful in similarity research and multiple regression analysis for the structure–property relationships. So, it is significant to generalize higher Wiener numbers and Wiener Matrices of acyclic structures to cyclic structures.

The present work, based on Klein–Lukovits–Gutman's definition [4] for the hyper-Wiener number, gives a new definition of higher Wiener numbers, so that it is applicable to any connected structure. The concepts of the Wiener vector and the hyper-Wiener vector of a graph are introduced. Moreover, by using the distance matrix $\mathbf{D} = \mathbf{D}(G)$ of a graph G, we introduce a Wiener matrix sequence (or distance matrix sequence) $\mathbf{W}^{(1)}, \mathbf{W}^{(2)}, \mathbf{W}^{(3)}, \ldots$, and their sum $\sum_{k=1,2,\cdots} \mathbf{W}^{(k)} = \mathbf{W}^{(H)}$, is called the hyper-Wiener matrix, where $\mathbf{W}^{(1)} = \mathbf{D}$ is the distance matrix, and the sum of the entries of the upper triangle of $\mathbf{W}^{(k)}$ (resp. $\mathbf{W}^{(H)}$) is just equal to ${}^kW$ (resp. R). A Wiener polynomial sequence and a weighted hyper-Wiener polynomial of a graph are also introduced.

Wiener Vectors and Hyper-Wiener Vectors

Klein et al. [4] derived a computationally efficacious formula for the hyper-Wiener number of a tree T by counting the number w'_{ij} of all subpaths in a path in T with end vertices i, j and length d_{ij}. Clearly, $w'_{ij} = \binom{d_{ij}+1}{2}$, and $R = \sum_{i<j} w'_{ij} = \sum_{i<j} w_{ij}$. However, the Klein–Lukovits–Gutman formula is applicable not only for trees but also for any connected cycle-containing structures.

According to Klein–Lukovits–Gutman's method, we can generalize the higher Wiener numbers as follows:

Definition 1. For a connected graph G with n vertices, denoted by 1, 2, . . . , n, let $w_{ij,k} = max\{d_{ij} - k + 1, 0\}$ where d_{ij} is the distance between vertices i and j. Then ${}^kW = \sum_{i<j} w_{ij,k}$, $k = 1, 2, \ldots$, are called the higher Wiener numbers of G. The vector (${}^1W$, ${}^2W, \cdots$) is called the hyper-Wiener vector of G, denoted by $HWV(G)$.

In Definition 1, $w_{ij,k}$ is just equal to the number of all subpaths of length k in a shortest path with end vertices i, j. If G is a tree, then ${}^kW = \sum_{i<j} w_{ij,k} =$

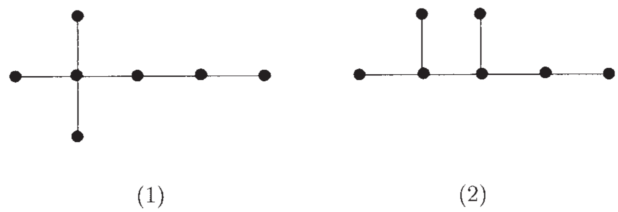

FIGURE 1. (1) A tree T_1, $W(T_1) = 46$, $WV(T_1) = (6, 16, 12, 12)$. (2) A tree T_2, $W(T_2) = 46$, $WV(T_2) = (6, 14, 18, 8)$.

$\sum_{d_{ij}=k,i<j} w_{ij}$, meaning that the new definition of the higher Wiener numbers of a connected graph is a natural extension of the higher Wiener numbers of a tree.

In addition, we have that the first component of the hyper-Wiener vector is equal to the Wiener number and the sum of all components of the vector is equal to the hyper-Wiener number, that is, ${}^1W = W$ and $\sum_{k=1,2,\cdots} {}^kW = \sum_{i<j} w'_{ij} = R$.

Similarly, we can introduce the Wiener vector of a graph G as follows:

Definition 2. For a connected graph G with n vertices, denoted by $1, 2, \ldots, n$, let $W_k = \sum_{i<j,d_{ij}=k} d_{ij}$, $k = 1, 2, \ldots$. The vector $(W_1, W_2, \cdots)$ is called the Wiener vector of G, denoted by $WV(G)$.

Clearly, the sum of all components of the Wiener vector of G is just equal to the Wiener number of G.

Figure 1 shows two trees T_1 and T_2, which have the same Wiener number but different Wiener vectors. This means that Wiener vectors have higher discrimination than do Wiener numbers.

For hyper-Wiener vectors, we believe that there are nonisomorphic graphs that have the same hyper-Wiener number but have different hyper-Wiener vectors. Such instances need to be found in the further investigation.

Wiener Matrix Sequences

Wiener matrix of a tree has not been generalized to cycle-containing structures. Based on the distance matrix of a graph, we will now introduce a Wiener matrix sequence (or distance matrix sequence) and hyper-Wiener matrix.

Definition 3. Let $\mathbf{D}$ be the distance matrix of a connected graph G. A Wiener matrix sequence $\mathbf{W}^{(1)}$, $\mathbf{W}^{(2)}$, $\mathbf{W}^{(3)}, \cdots$ is defined as follows:

1. Let $\mathbf{W}^{(1)} = \mathbf{D}$.
2. For $k = 1, 2, \ldots$, $\mathbf{W}^{(k+1)}$ is obtained from $\mathbf{W}^{(k)}$ by leaving zeroes in place and replacing each nonzero entry x of $\mathbf{W}^{(k)}$ by $x - 1$.

Definition 4. Let $\mathbf{D}$ be the distance matrix of a connected graph G, and let $\mathbf{W}^{(1)}, \mathbf{W}^{(2)}, \mathbf{W}^{(3)}, \cdots$ be the Wiener matrix sequence of G. The hyper-Wiener matrix $\mathbf{W}^{(H)}$ of G is then defined as $\mathbf{W}^{(H)} = \sum_{k=1,2,\cdots} \mathbf{W}^{(k)}$.

From the above definitions, we can see that (i, j)-entry of $\mathbf{W}^{(k)}$ is just equal to $d_{ij} - k + 1$, so the sum of entries of upper triangle of $\mathbf{W}^{(k)}$ is just equal to ${}^kW$. Moreover, the sum of entries of upper triangle of the hyper-Wiener matrix $\mathbf{W}^{(H)}$ is just equal to the hyper-Wiener number R.

Note that the sum of entries of the upper triangle of the Wiener matrix of a tree is also equal to the hyper-Wiener number. However, the hyper-Wiener matrix is applicable not only to trees, but also for any connected structure.

For graph G in Figure 2, its Wiener matrix sequence, Wiener vector, and hyper-Wiener vector can be shown as follows:

$$W^{(1)} = \begin{pmatrix} 0 & 1 & 2 & 3 & 2 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 \end{pmatrix},$$

$$W^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 2 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 \\ 1 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 \end{pmatrix},$$

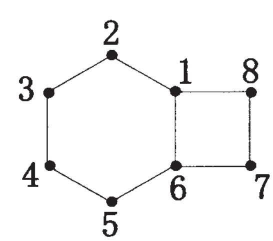

FIGURE 2. Graph G.

$$W^{(3)} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \end{pmatrix},$$

$$W^{(4)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$W^{(H)} = \begin{pmatrix} 0 & 1 & 3 & 6 & 3 & 1 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 3 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 \\ 3 & 6 & 3 & 1 & 0 & 1 & 3 & 6 \\ 1 & 3 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 \\ 1 & 3 & 6 & 10 & 6 & 3 & 1 & 0 \end{pmatrix},$$

$WV(G) = (9, 20, 21, 8)$, $HWV(G) = (58, 30, 11, 2)$, $W = 58$, $R = 101$.

Wiener Polynomial Sequence and Hyper-Wiener Polynomial

The Wiener polynomial of graph was first introduced by Hosoya [21]. Let D be the distance matrix of a graph G, let l be the largest entry of D, and let $2d_k$ be the number of such entries of D that are equal to k. The Wiener polynomial $W(G, x)$ of G is then given by

$$W(G, x) = \sum_{k=1}^{l} d_k x^k.$$

Later Sagan and Yeh and colleagues [22, 23] defined a generating function $W(G, x)$ related to the Wiener index of a graph G, called the Wiener polynomial:

$$W(G, x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)},$$

where $d(u, v)$ denotes the distance between vertices u and v.

The above two formulae give the same polynomial of G, in fact.

It was shown in Refs. [19, 21–23] that

$$W = W'(G, 1), \qquad R = W'(G, 1) + \tfrac{1}{2} W''(G, 1).$$

In Ref. [19], Cash introduced a new hyper-Hosoya polynomial $HH(G, x) = \sum_{k=0}^{l} [(k + 1)/2]\, d_k x^k$, and showed that $R(G) = HH'(G, 1)$.

It can be found that the Wiener vector $(W_1, W_2, \cdots)$ consists of the coefficients of the derivative $W'(G, x)$ of the Wiener polynomial, where W_k is equal to the coefficient kd_k of x^{k-1} in $W'(G, x)$. However, the hyper-Wiener vector cannot be obtained from the hyper Hosoya polynomial $HH(G, x)$.

In a hyper-Wiener vector, ${}^1W = W$, so we can call ${}^1W = W$ the first Wiener number and ${}^kW$ the kth Wiener number. According to the Wiener polynomial, we will introduce a Wiener polynomial sequence $W_1(G, x)$, $W_2(G, x)$, $W_3(G, x)$, $\cdots$ of a graph G, where the kth Wiener polynomial of G is closely related to the kth Wiener number.

Definition 5. Let G be a connected graph with n vertices. The kth Wiener polynomial of G, $1 \leq k \leq dia(G)$, is defined by $W_k(G, x) = \sum_{\{u,v\} \subset V(G)} x^{\max\{d(u,v)-k+1,0\}}$, where dia($G$) is the diameter of G. The polynomial sequence $W_1(G, x)$, $W_2(G, x)$, $W_3(G, x)$, $\cdots$ is called the Wiener polynomial sequence of G.

It is not difficult to verify that $W_1(G, x) = W(G, x)$ and $W'_k(G, 1) = {}^kW$. The constant term of $W_k(G, x)$ is equal to the number of the pairs of vertices with distances less than k.

For the hyper-Wiener vector of a graph G, its components ${}^iW$ and ${}^jW$ might have different contributions in some research for the structure–property relationship. We can weight the kth Wiener number by y_k and define a weighted hyper-Wiener number as follows.

Definition 6. The weighted hyper-Wiener number $R_W(G)$ of a graph G is defined as $R_W(G) = \sum_{k=1,2,\cdots} {}^kW y_k$, where y_k is the weight of ${}^kW$.

In addition, we will introduce a novel weighted hyper-Wiener polynomial $HW(G, x, y)$ of a graph G, so that the hyper-Wiener vector and the weighted hyper-Wiener number can be obtained from the polynomial.

Definition 7. The weighted hyper-Wiener polynomial $HW(G, x, y)$ of a graph G is defined as $HW(G, x, y) = \sum_{k=1,2,\cdots} W_k(G, x) \cdot y_k$, where $y = (y_1, y_2, \cdots)$.

From Definition 7, we have that

$$\frac{d}{dx}[HW(G, x, y)]|_{x=1} = \sum_{k=1,2,\ldots} {}^kWy_k = R_W(G),$$

where the coefficients of y_k in the weighted hyper-Wiener number $R_W(G)$ are equal to the kth Wiener number. Hence, the hyper-Wiener vector can be given by coefficients of $(d/dx)[HW(G, x, y)]|_{x=1}$. In particular, we have that

$$\frac{d}{dx}[HW(G, x, y)]|_{x=1,y=(1,1,1,\ldots)} = R(G).$$

For graph G in Figure 2, the Wiener vector, the Wiener polynomial sequence, the weighted hyper-Wiener polynomial of G can be given as follows:

$$W'(G, x) = 8x^3 + 21x^2 + 20x + 9,$$

$$WV(G) = (9, 20, 21, 8),\ W(G) = 58.$$

$$W^{(1)}(G, x) = 2x^4 + 7x^3 + 10x^2 + 9x,$$

$$W^{(2)}(G, x) = 2x^3 + 7x^2 + 10x + 9,$$

$$W^{(3)}(G, x) = 2x^2 + 7x + 19,$$

$$W^{(4)}(G, x) = 2x + 26.$$

$$HW(G, x, y) = (2x^4 + 7x^3 + 10x^2 + 9x)y_1 + (2x^3 + 7x^2 + 10x + 9)y_2 + (2x^2 + 7x + 19)y_3 + (2x + 26)y_4.$$

$$\frac{d}{dx}[HW(G, x, y)]|_{x=1} = 58y_1 + 30y_2 + 11y_3 + 2y_4,$$

$$HWV(G) = (58, 30, 11, 2),$$

$$\frac{d}{dx}[HW(G, x, y)]|_{x=1,y=(1,1,1,\cdots)} = R(G) = 101.$$

From the above example, it can be found that if the kth Wiener polynomial is given, the $(k + 1)$th Wiener polynomial can be obtained from $W^{(k)}(G, x)$ by replacing exponent k of x^k by $k - 1$ for $k = 1, 2, \ldots$.

Discussion

In the present work, we have generalized the Wiener matrix and the higher Wiener numbers of a tree to cyclic structures, and introduce a series of novel topological invariants such as the Wiener vector, the hyper-Wiener vector, the Wiener matrix sequence, the Wiener polynomial sequence, the weighted hyper-Wiener number, and the weighted hyper-Wiener polynomial for any connected structure. They will be useful in similarity research and multiply regression analysis for structure-property relationship. There are some open problems for further investigation. We list some as follows.

Problem 1: Find the minimum nonisomorphic graphs (trees or cycle-containing structures), which have the same hyper-Wiener number but different hyper-Wiener vectors.

Problem 2: Find the minimum non-isomorphic graphs (trees or cycle-containing structures), which have the same hyper-Wiener vector but different hyper-Wiener matrices or different Wiener matrix sequences.

[Here, two matrices different mean that they cannot be transformed by simultaneous permutations on rows and columns.]

Problem 3: Properties of the new topological invariants with application in structure–property relationship research and similarity research.

Problem 4: Properties and calculation methods of spectrums of the new matrices and properties of roots of the new polynomials.

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