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q-Analog of Wiener Index

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Abstract

The Wiener index is the sum of distances between all pairs of vertices of a connected graph. In this paper we propose q-analogs of the Wiener index, motivated by the theory of hypergeometric series. The basic properties of these q-Wiener indices are established, as well as their relations with the Hosoya polynomial. Some possible chemical interpretations and applications of the q-Wiener indices are considered.

1 Introduction

In this paper we are concerned with simple graphs, and all graphs considered are assumed to be connected. Let G be such a graph, with $V(G)$ and $E(G)$ being its vertex and edge sets, respectively. The number of vertices of G, i. e., $|V(G)|$, is denoted by $n = n(G)$.

The distance between two vertices u and v, denoted by $d(v, u)$, is the length of a shortest path between v and u. Then the Wiener index of G is

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

which also could be written as

$$W = W(G) = \sum_{k \geq 1} k \, d(G,k) \tag{1}$$

where $d(G,k)$ is the number of pairs of vertices of the graph G whose distance is k.

For details of the mathematical theory of the Wiener index and its chemical applications see [1–4]; for some recent works along these lines see [5–10].

The aim to this paper is to study the q-analog of the Wiener index. The earliest q-analog studied in detail is the basic hypergeometric series, which was introduced in the 19th century [11].

A q-analog is, roughly speaking, a theorem or identity in the variable q that gives back a known result in the limit, as $q \to 1$ (from inside the complex unit circle in most situations).

q-Analogs find applications in a number of areas, including the study of fractals and multi-fractal measures, and expressions for the entropy of chaotic dynamic systems. q-Analogs also appear in the study of quantum groups and in q-deformed superalgebras [12, 13].

2 Definitions and Basic Properties

2.1 q-Wiener index

Let q be a positive real number, $q \neq 1$. We define the q-analog of k, also known as the q-bracket or q-number of k, to be

$$[k]_q = \frac{1-q^k}{1-q} = \sum_{0 \leq i < k} q^i = 1 + q + q^2 + \cdots + q^{k-1} \; . \tag{2}$$

Then $\lim_{q \to 1} [k]_q = k$.

Based on this formalism, one can conceive the q-analog of the Wiener index as

$$W_1(G,q) = \sum_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \; .$$

In what follows we shall also consider the second and third q-analogs of W, defined as

$$\begin{aligned} W_2(G,q) &= \sum_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \, q^{L-d(v,u)} \\ W_3(G,q) &= \sum_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \, q^{d(v,u)} \end{aligned}$$

where L is the diameter of G. Again, one recovers the usual Wiener index by taking the limit $q \to 1$:

$$\lim_{q\to 1} W_1(G,q) = \lim_{q\to 1} W_2(G,q) = \lim_{q\to 1} W_3(G,q) = W(G)\ . \tag{3}$$

It is evident that such a generalization of the Wiener–index concept can be further extended by considering

$$\sum_{\{v,u\}\subseteq V(G)} [d(v,u)]_q\, \Phi(q, d(v,u))$$

with $\Phi(x,y)$ being any function in the variables x and y, such that $\lim\limits_{x\to 1} \Phi(x,y) = 1$ for all values of y. Yet we stop at W_1, W_2, and W_3.

Bearing in mind Eqs. (1) and (2), it is straightforward to show that

$$W_1(G,q) = \sum_{k\geq 1} [k]_q\, d(G,k) = \sum_{k\geq 1} (1+q+q^2+\cdots+q^{k-1})\, d(G,k) \tag{4}$$

$$W_2(G,q) = \sum_{k\geq 1} [k]_q\, q^{L-k}\, d(G,k) = \sum_{k\geq 1} (1+q+q^2+\cdots+q^{k-1})\, q^{L-k}\, d(G,k) \tag{5}$$

$$W_3(G,q) = \sum_{k\geq 1} [k]_q\, q^k\, d(G,k) = \sum_{k\geq 1} (1+q+q^2+\cdots+q^{k-1})\, q^k\, d(G,k)\ . \tag{6}$$

In addition, we have the following relations among the three q-Wiener indices:

$$\begin{aligned} W_1(G,q) &= q^{L-1}\, W_2\left(G, \frac{1}{q}\right) \\ W_2(G,q) &= q^{L-1}\, W_1\left(G, \frac{1}{q}\right) \\ W_3(G,q) &= (1+q)\, W_1(q^2) - W_1(G,q)\ . \end{aligned}$$

Let v and u be two vertices of the graph G and let their distance be d. The shortest path between v and u can be viewed as a sequence d mutually incident edges, $e_1, e_2, \ldots, e_d$, such that v is an end-vertex of e_1 and u and end-vertex of e_d. So, we can go from v to u in d steps, along the edges $e_1, e_2, \ldots, e_d$. Suppose that the contribution of the first step is unity, of the second step is q, of the third step q^2, of the i-th step is q^{i-1}. The contribution obtained by moving along the entire shortest path would then be $1+q+q^2+\cdots+q^{d-1}$. This observation may serve for an interpretation of the invariants W_1, and after an obvious modification, also of W_2 and W_3. If the parameter q is chosen to be positive and less than unity, then the q-analogs of the Wiener index would provide models for measuring interactions between individual atoms in a molecule which are known to decrease with their distance.

In connection with the above deliberations, it should be mentioned that in a recent paper [14], a class of invariants of (molecular) graphs was considered, having the form

$$\tilde{Q} = \sum_{\{v,u\} \subseteq V(G)} f(d(v,u))$$

where $f(x)$ depends solely on the distance d(u,v) between the vertices u and v. This invariant satisfies the identity

$$\tilde{Q} = \sum_{k \geq 1} f(k)\, d(G,k)$$

which should be compared with Eqs. (1) and (4)–(6).

Adopting the standard convention

$$\sum_{k=m}^{n} a_k = \begin{cases} a_m + a_{m+1} + \cdots + a_n & \text{if } m \leq n \\ 0 & \text{if } m = n+1 \end{cases}$$

by straightforward calculation we arrive at:

Proposition 1. *The q-Wiener indices $W_1(G,q)$, $W_2(G,q)$, and $W_3(G,q)$ are polynomials in q, and*

$$\begin{aligned} W_1(G,q) &= \sum_{k=0}^{L-1} \sum_{j=k+1}^{L} d(G,j)\, q^k && (7) \\ W_2(G,q) &= \sum_{k=0}^{L-1} \sum_{j=0}^{k} d(G,L-k+j)\, q^k \\ W_3(G,q) &= \sum_{k=0}^{L-1} \sum_{j=\lfloor k/2 \rfloor+1}^{k} d(G,j)\, q^k + \sum_{k=L}^{2L-1} \sum_{j=\lfloor k/2 \rfloor+1}^{L} d(G,j)\, q^k \end{aligned}$$

where $\lfloor \ell \rfloor$ is the greatest integer smaller or equal to ℓ.

This proposition shows us that the coefficients of q^k in $W_1(G,q)$, $W_2(G,q)$, and $W_3(G,q)$ is exactly the numbers of edges of G that have been weighted with q^k.

In Table 1 are given the coefficients of the polynomial $W_1(G,q)$ for some alkanes, according to Eq. (7).

alkane	a_0	a_1	a_2	a_3	a_4	a_5	a_6	$W(G)$
2-methyloctane	36	28	20	14	9	5	2	114
3-methyloctane	36	28	20	13	8	4	1	110
4-methyloctane	36	28	20	13	7	3	1	108
2,2-dimethyloctane	45	36	25	18	12	7	3	146
2,3-dimethyloctane	45	36	26	17	11	6	2	143
2,4-dimethyloctane	45	36	26	18	10	5	2	142
3,3-dimethyloctane	45	36	25	16	10	5	1	138
3,4-dimethyloctane	45	36	26	16	9	4	1	137
4,4-dimethyloctane	45	36	25	16	8	3	1	134
2,2,3-trimethyloctane	55	45	32	21	14	8	3	178
2,2,4-trimethyloctane	55	45	32	23	13	7	3	178
2,3,3-trimethyloctane	55	45	32	20	13	7	2	174
2,3,4-trimethyloctane	55	45	33	21	12	6	2	174
3,3,4-trimethyloctane	55	45	32	19	11	5	1	168
3,4,4-trimethyloctane	55	45	32	19	10	4	1	166
2,2,4,4-tetramethyloctane	66	55	39	28	14	7	3	212
2,3,4,5-tetramethyloctane	66	55	41	26	14	6	2	210

Table 1. The coefficients a_k $(0 \leq k \leq 6)$, pertaining to q^k in Eq. (7).

From Table 1 we see that $2,2,3$-trimethyloctane and $2,2,4$-trimethyloctane have equal Wiener indices $W(G)$, but different $W_1(G,q)$. The same is true for $2,3,3$-trimethyloctane and $2,3,4$-trimethyloctane. This hints toward possible advantages of the q-Wiener indices over the ordinary Wiener index.

The vast majority of chemical applications of the Wiener index deal with acyclic organic molecules. Their molecular graphs are trees [15]. In view of this, it is not surprising that in the chemical literature there are numerous studies of properties of the Wiener indices of trees.

A tree is a connected acyclic graph. Each pair of vertices of a tree is connected by a unique path. A vertex of degree one is called a pendent vertex. A tree on n vertices has at least 2 and at most $n-1$ pendent vertices. The (unique) n-vertex trees with 2 and $n-1$ pendent vertices are the path and the star, respectively, denoted by P_n and S_n, respectively. For these trees we have:

Proposition 2. *For $n \geq 2$,*

$$\begin{aligned}
W_1(S_n,q) &= \binom{n}{2} + \binom{n-1}{2} q \\
W_2(S_n,q) &= \binom{n-1}{2} + \binom{n}{2} q \\
W_3(S_n,q) &= (n-1)q + \binom{n-1}{2} q^2 + \binom{n-1}{2} q^3 \\
W_1(P_n,q) &= \binom{n}{2} + \binom{n-1}{2} q + \binom{n-2}{2} q^2 + \cdots + q^{n-2} \\
W_2(P_n,q) &= 1 + \binom{3}{2} q + \binom{4}{2} q^2 + \cdots + \binom{n}{2} q^{n-2} \\
W_3(P_n,q) &= \sum_{k=1}^{n-2} \frac{1}{2} \left(2n - k - \left\lfloor \frac{k}{2} \right\rfloor - 1\right) \left(k - \left\lfloor \frac{k}{2} \right\rfloor\right) q^k + \sum_{k=n-1}^{2n-3} \binom{n - \lfloor \frac{k}{2} \rfloor}{2} q^k \; .
\end{aligned}$$

2.2 q-Multiplicative Wiener index

Few years ago the multiplicative version of the Wiener index, denoted by $\pi(G)$, was put forward [16]. This molecular structure descriptor is equal to the product of the distances of all pairs of vertices of the underlying molecular graph, i. e.,

$$\pi(G) = \prod_{\{v,u\} \subseteq V(G)} d(v,u) \; .$$

Since this index is, even for small molecular graphs, rather large number, e. g. 34,560 for the hexane graph (P_6), in QSPR/QSAR modeling it is convenient to work with $\log \pi(G)$ instead of $\pi(G)$. Of course,

$$\log \pi(G) = \sum_{\{v,u\} \subseteq V(G)} \log d(v,u) = \sum_{k \geq 1} (\log k)\, d(G,k) \; .$$

The q-analogs of the multiplicative Wiener index are defined in full analogy with $W_i(G,q)$, $i = 1,2,3$:

$$\begin{aligned}
\pi_1(G,q) &= \prod_{\{v,u\} \subseteq V(G)} [d(v,u)]_q = \prod_{k \geq 1} \{[k]_q\}^{d(G,k)} \\
\pi_2(G,q) &= \prod_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \, q^{L-d(v,u)} = \prod_{k \geq 1} \{[k]_q \, q^{L-k}\}^{d(G,k)} \\
\pi_3(G,q) &= \prod_{\{v,u\} \subseteq V(G)} [d(v,u)]_q \, q^{d(v,u)} = \prod_{k \geq 1} \{[k]_q \, q^k\}^{d(G,k)}
\end{aligned}$$

from which it immediately follows:

$$\log \pi_1(G,q) = \sum_{k\geq 1} \left(\log \frac{1-q^k}{1-q} \right) d(G,k)$$

$$\log \pi_2(G,q) = \sum_{k\geq 1} \left(\log \frac{1-q^k}{1-q} \right) d(G,k) + \binom{n}{2} L \log q - W(G) \log q$$

$$\log \pi_3(G,q) = \sum_{k\geq 1} \left(\log \frac{1-q^k}{1-q} \right) d(G,k) + W(G) \log q \; .$$

3 Relations between q-Wiener Indices and Hosoya Polynomial

The counting polynomial

$$H(G,\lambda) = \sum_{k=1}^{L} d(G,k)\, \lambda^k \tag{8}$$

was first put forward by Hosoya [17]. Hosoya himself called it "*Wiener polynomial*", but eventually the more appropriate name "*Hosoya polynomial*" has been accepted.

Combining Eq. (8) with the definitions of the q-Wiener indices, we arrive at:

Proposition 3. *Let G be a connected graph on n vertices. Then*

$$W_1(G,q) = \frac{1}{1-q} \left[\binom{n}{2} - H(G,q) \right]$$

$$W_2(G,q) = \frac{q^L}{1-q} \left[H\left(G, \frac{1}{q}\right) - \binom{n}{2} \right]$$

$$W_3(G,q) = \frac{1}{1-q} \left[H(G,q) - H(G,q^2) \right].$$

The most famous property of the Hosoya polynomial is that its first derivative at $\lambda = 1$ is equal to the Wiener index [17]. The analogous relations between the derivatives of the q-Wiener indices and the Hosoya polynomial are stated in:

Proposition 4. *Let G be a connected graph. Then,*

$$W_1'(G,q) = \frac{1}{1-q} \left[W_1(G,q) - H'(G,q) \right]$$

$$W_2'(G,q) = \frac{1}{1-q} \left\{ W_2(G,q) + L\, q^{L-1} \left[H\left(G, \frac{1}{q}\right) - \binom{n}{2} \right] - q^{L-2}\, H'\left(G, \frac{1}{q}\right) \right\}$$

$$W_3'(G,q) = \frac{1}{1-q} \left[W_3(G,q) + H'(G,q) - 2qH'(G,q^2) \right] \; .$$

By taking the limit $q \to 1$, we get:

$$\begin{aligned}
W_1'(G,1) &= \frac{1}{2}\,H''(G,1)\\
W_2'(G,1) &= \frac{1}{2}\left[(2L-2)H'(G,1) - H''(G,1)\right]\\
W_3'(G,1) &= \frac{1}{2}\left[2H'(G,1) + 3H''(G,1)\right]\,.
\end{aligned}$$

Before stating the next properties, we need to define the partial Hosoya polynomial $H_m(G,\lambda)$, defined as

$$\begin{aligned}
&H_m(G,\lambda) \equiv 0 && \text{if } m = 0\\
&H_m(G,\lambda) = \sum_{k=1}^{m} d(G,k)\,\lambda^k && \text{if } m = 1,2,3,\ldots,L\,.
\end{aligned}$$

We see that $H_L(G,\lambda) = H(G,\lambda)$ and $H_L(G,1) = \binom{n}{2}$.

Proposition 5. *Let G be a connected graph. Then,*

$$\begin{aligned}
W_1(G,q) &= \sum_{k=0}^{L-1}\left[H_L(G,1) - H_k(G,1)\right] q^k\\
W_2(G,q) &= \sum_{k=0}^{L-1}\left[H_L(G,1) - H_{L-k-1}(G,1)\right] q^k\\
W_3(G,q) &= \sum_{k=0}^{2L-1}\left[H_L(G,1) - H_{\lfloor k/2\rfloor}(G,1)\right] q^k - \sum_{k=0}^{L-1}\left[H_L(G,1) - H_k(G,1)\right] q^k\,.
\end{aligned}$$

Bearing in mind the limit values (3), we arrive at the following interesting corollary of Proposition 5:

$$W(G) = \sum_{k=0}^{L-1}\left[H_L(G,1) - H_k(G,1)\right]\,.$$

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