Wiener Indices and Polynomials of Five Graph Operators

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Abstract

The sum of distances between all vertices pairs in a connected graph is known as the *Wiener Index*. It is the earliest of the *indices* that correlates well with many physico-chemical properties of organic compounds and as such has been well-studied over the last quarter of a century. A q-analogue of this index, termed the *Wiener Polynomial* by Hosoya but also known today as the *Hosoya Polynomial*, extends this concept by trying to capture the complete distribution of distances in the graph.

The mathematicians have studied several operators on a connected graph in which we see a subdivision of the edges. Herein we show how the Wiener Index of a graph changes with these operations, and extend the results to Wiener Polynomials.

Keywords: Wiener Index, Subdivision, Line graph, Total graph, Wiener Polynomial.

1 Introduction

We hereby introduce the Wiener Index and Polynomial on connected graphs. Chemists use many quantities associated with a molecular graph to estimate various physical properties (see, for example, [1, 2, 3, 9]). One of the eldest of these is the Index of Harold Wiener, defined in 1947 [4].

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Definition 1 *The **Wiener Index** [4] and **Polynomial** [5, 6] of a connected graph G are*

$$\mathcal{W}(G;q) := \sum_{\{u,v\}\subset V(G)} q^{d_G(u,v)}, \quad \mathcal{W}(G) := \sum_{\{u,v\}\subset V(G)} d_G(u,v) = \left.\frac{d\mathcal{W}(G;q)}{dq}\right|_{q=1},$$

where $d_G(u,v)$ denotes the distance between two vertices u and v in G.

For example, $\mathcal{W}(G) = 40$ and $\mathcal{W}(G;q) = q^4 + 4q^3 + 8q^2 + 8q$ for the graph G illustrated in Fig. 1(a).

The Wiener Polynomial is initially defined by Haruo Hosoya [5], and so termed in honour of Harold Wiener who coined the earlier index. It is often called the Hosoya Polynomial and appears in slightly different forms in the literature. The readers interested in the continuing saga of Wiener Indices and Polynomials will have to refer to a dedicated survey (see, for example, [10, 5, 6]).

2 Subdivision Operators

Suppose $G = (V, E)$ is a connected graph with the vertex set V and the edge set E. Give an edge $e = (u, v)$ of G, let $V(e) = \{u, v\}$. Now we can define the following related graphs: the *line graph* $L(G)$, the *subdivision* $S(G)$, the *total graph* $T(G)$ as follows (see, for example, [7]):

Line Graph: $L(G)$ is the graph whose vertices correspond to the edges of G with two vertices being adjacent if and only if the corresponding edges in G have a vertex in common (see Fig. 1(b)).

Subdivision Graph: $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two, or equivalently, by inserting an additional vertex into each edge of G (see Fig. 1(c)).

Total Graph: $T(G)$ is the graph whose vertex set is $V \cup E$, with two vertices of $T(G)$ being adjacent if and only if the corresponding elements of G are adjacent or incident (see Fig. 1(d)).

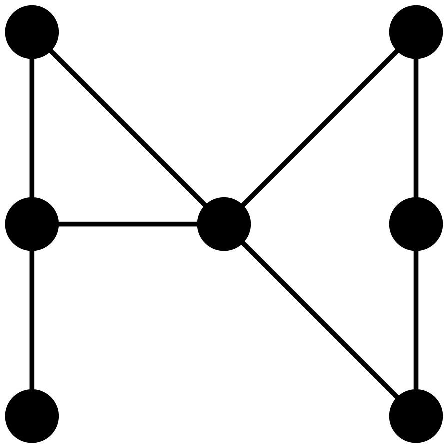
Two extra subdivision operators named $R(G)$ and $Q(G)$ (following the notations [7] that does not give the structures any specific names.) are defined as follows:

$R(G)$ is defined as the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it (see Fig. 2).

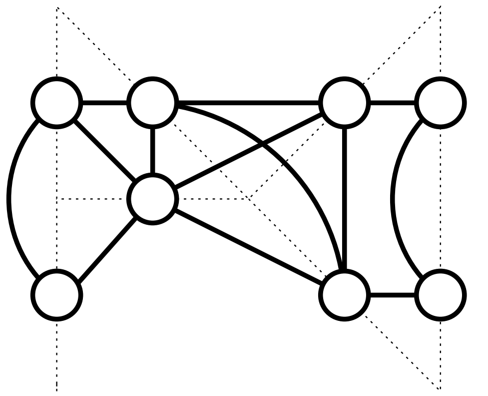
$Q(G)$ is the graph obtained from G by inserting a new vertex into each edge of G and by joining edges those pairs of these new vertices which lie on adjacent edges of G (see Fig. 2).

Given $G = (V, E)$, where $E \subset \binom{V}{2}$, we may define two other sets that we use frequently:

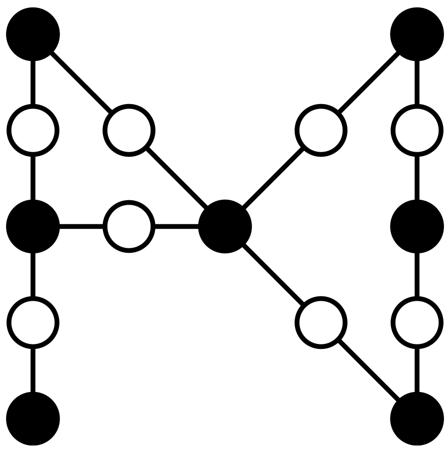
$$\begin{aligned} EE(G) &:= \{\{e, e'\} : e, e' \in E(G),\, e \neq e',\, |V(e) \cap V(e')| = 1\}. \\ EV(G) &:= \{\{e, v\} : V(G) \ni v \in V(e), e \in E(G)\}. \end{aligned}$$



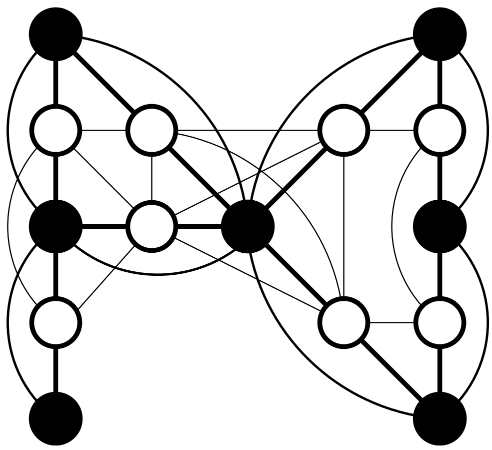
(a) Original Graph G



(b) Line Graph $L(G)$

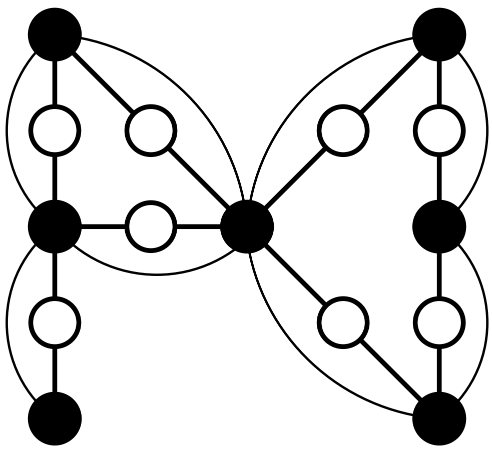


(c) Subdivision $S(G)$

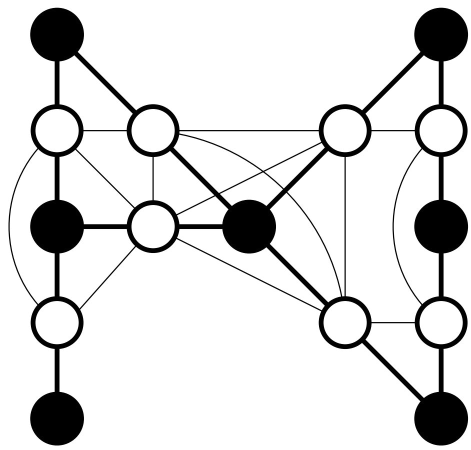


(d) Total Graph $T(G)$

Figure 1: The common Subdivision operators S and T



(a) $R(G)$



(b) $Q(G)$

Figure 2: The two additional subdivision operators

We may then write the subdivision operators above as follows:

$$\begin{aligned}
L(G) &:= (E(G),\, EE(G)),\\
S(G) &:= (V(G)\cup E(G),\, EV(G)),\\
T(G) &:= (V(G)\cup E(G),\, E(G)\cup EV(G)\cup EE(G)),\\
R(G) &:= (V(G)\cup E(G),\, EV(G)\cup E(G)),\\
Q(G) &:= (V(G)\cup E(G),\, EV(G)\cup EE(G)),
\end{aligned}$$

As early as in 1981 Buckley [8] investigated the relation between the Wiener index of a tree T and its line graph $L(T)$ and established a quite simple result as follows:

$$W(L(T)) = W(T) - \binom{n}{2}.$$

This is perhaps the first result considered the relations between the Wiener indices of a graph and its graph operator. In this paper, we will in the next section outline our results on Wiener indices of these subdivision graphs, and proceed to prove them and move on to Wiener Polynomials.

3 Distances in Subdivision Graphs and Their Wiener Indices

Let G be a connected graph. That $e, e' \in E(G)$, *are connected as vertices in* $L(G)$, $T(G)$ *or* $Q(G)$ will be marked $e \stackrel{e\cap e'}{\rightarrow} e'$. In other words, If $e = \{v, v'\}$ and $e' = \{v, v''\}$, then we will write $e \stackrel{v}{\rightarrow} e'$ even though the edge is technically $\{e, e'\}$.

Lemma 1 *For any* $v, v' \in V(G)$,

$$\frac{1}{2} d_{S(G)}(v, v') = d_{T(G)}(v, v') = d_{R(G)}(v, v') = d_{Q(G)}(v, v') - 1 = d_G(v, v')$$

Proof. Let the short path (of length k) in G from v to v' be represented by the sequence

$$v = v_0 \stackrel{e_1}{\rightarrow} v_1 \stackrel{e_2}{\rightarrow} v_2 \cdots \stackrel{e_k}{\rightarrow} v_k = v'.$$

1. The same path also represents the shortest distance in $T(G)$ and $R(G)$. In the latter, one can only get from edge to edge through a vertex, and the path $u \rightarrow p \rightarrow u'$ can always be shortened to $u \stackrel{p}{\rightarrow} u'$. In the former, the segment of a path that proceeds

   $$u = u_0 \rightarrow p_0 \stackrel{u_1}{\rightarrow} p_1 \stackrel{u_2}{\rightarrow} p_2 \cdots \stackrel{u_\ell}{\rightarrow} p_\ell \rightarrow u_{\ell+1}$$

   of length $(\ell + 2)$ can always be replaced by the following segment of length $(\ell + 1)$:

   $$u = u_0 \stackrel{p_0}{\rightarrow} u_1 \stackrel{p_1}{\rightarrow} u_2 \stackrel{p_2}{\rightarrow} \cdots u_\ell \stackrel{p_\ell}{\rightarrow} u_{\ell+1}.$$

   Here u's are vertices of G and p's are edges of G. Now we know that shortest paths between vertices of G in $T(G)$ and $R(G)$ only visits other vertices of G (as vertices!). hence what was a shortest path in G would remain so in $T(G)$ and $R(G)$.

2. The shortest distance in $S(G)$ from v to v' is clearly represented by

$$v = v_0 \to e_1 \to v_1 \to e_2 \to v_2 \cdots \to e_k \to v_k = v',$$

as one can only alternate between the vertices and edges of G when traversing $S(G)$.

3. In $Q(G)$, to get from one vertex of G to another it is necessary to go through at least one edge of G (consider as a vertex here!). Furthermore, any $p \to u \to p'$ segment can be shortened to $p \stackrel{u}{\to} p'$. Since any path

$$v = u_0 \to p_0 \stackrel{u_1}{\to} p_1 \stackrel{u_1}{\to} p_2 \cdots \stackrel{u_{\ell-1}}{\to} p_\ell \to u_l = v'$$

of length $\ell + 1$ in $Q(G)$ corresponds to the path

$$v = u_0 \stackrel{p_0}{\to} u_1 \stackrel{p_1}{\to} u_2 \stackrel{p_2}{\to} \cdots u_{\ell-1} \stackrel{p_\ell}{\to} u_\ell = v'$$

of length ℓ in G. The shortest path in in $Q(G)$ from v to v' is hence

$$v_0 \to e_1 \stackrel{v_1}{\to} e_2 \stackrel{v_2}{\to} \cdots e_k \to v_k.$$

So we have proved all of Lemma 1. □

There are two other analogous lemmas for pairs of edges and edge-vertex pairs:

Lemma 2 *For any* $e, e' \in E(G)$

$$\frac{1}{2} d_{S(G)}(e, e') = d_{T(G)}(e, e') = d_{R(G)}(e, e') - 1 = d_{Q(G)}(e, e') = d_{L(G)}(e, e')$$

Proof. Let the short path (of length k) in $L(G)$ from e to e' be represented by the sequence

$$e = e_0 \stackrel{v_1}{\to} e_1 \stackrel{v_2}{\to} e_2 \cdots \stackrel{v_k}{\to} e_k = e'.$$

Then it will be shortest path between e and e' in $Q(G)$ and $T(G)$ (similar to point 3 of Lemma 1). In contrast, as in point 2 of Lemma 1, the shortest path in $S(G)$ will be

$$e = e_0 \to v_1 \to e_1 \to v_2 \to e_2 \cdots \to v_k \to e_k = e'.$$

i.e., of length $2k$. Finally, as in point 1 above, the shortest path (of length $k + 1$) in $R(G)$ is $e = e_0 \to v_1 \stackrel{e_1}{\to} v_2 \stackrel{e_2}{\to} \cdots v_k \to e_k = e'$. □

Lemma 3 *For any* $e \in E(G)$, $v \in V(G)$,

$$\frac{1}{2} \left(d_{S(G)}(e, v) + 1 \right) = d_{T(G)}(e, v) = d_{R(G)}(e, v) = d_{Q(G)}(e, v)$$

Proof. Assume that a shortest path of length $2k-1$ in $S(G)$ to be

$$e = e_1 \to v_1 \to e_2 \to v_2 \to e_3 \cdots \to v_{k-1} \to e_k \to v_k = v.$$

Similar arguments as point 3 of lemma 1 shows that the shortest path in $Q(G)$ (of length k) is

$$e = e_1 \stackrel{v_1}{\to} e_2 \stackrel{v_2}{\to} e_3 \cdots \stackrel{v_{k-1}}{\to} e_k \to v_k = v.$$

while point 1 above says the shortest path in $R(G)$ will be instead (also of length k):

$$e = e_1 \to v_1 \stackrel{e_2}{\to} v_2 \stackrel{e_3}{\to} \cdots v_{k-1} \stackrel{e_k}{\to} v_k = v.$$

And the shortest path in $T(G)$ can be either of the above. $\square$

Almost immediately we can prove some interesting relationships between various subdivisions:

Theorem 4 *If the connected graph G has m edges and n vertices, then*

$$\begin{aligned} \mathcal{W}(S(G)) &= 2\mathcal{W}(T(G)) - mn \\ \mathcal{W}(R(G)) &= \mathcal{W}(T(G)) + m(m-1)/2 \\ \mathcal{W}(Q(G)) &= \mathcal{W}(T(G)) + n(n-1)/2 \end{aligned}$$

Proof. Split the sum over 2-subsets $\{x, x'\}$ of $E(G) \cup V(G)$ three ways into sums over $\{v, v'\} \in \binom{V(G)}{2}$, $\{e, e'\} \in \binom{E(G)}{2}$, and $(e \in E(G), v \in V(G))$, then use Lemmas 1—3. $\square$

Remark: We may eliminate $T(G)$ for a relation between the Wiener indices of $S(G), R(G), Q(G)$:

$$\mathcal{W}(S(G)) = \mathcal{W}(R(G)) + \mathcal{W}(Q(G)) + \binom{m+n}{2}.$$

4 Wiener Polynomials of Subdivision Graphs

We may observe that there are other ways we can use the lemmas in the above section. E.g., we may derive connections between Wiener (Hosoya) Polynomials of subdivided graphs:

Theorem 5 *For a connected graph G, we have*

$$\mathcal{W}(S(G); q) = \frac{1}{q}\,\mathcal{W}(T(G); q^2) + \left(1 - \frac{1}{q}\right)\left[\mathcal{W}(G; q^2) + \mathcal{W}(L(G); q^2)\right] \tag{1}$$

Proof.

$$
\begin{aligned}
\mathcal{W}(S(G);q) &= \sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{d_{S(G)}(v,v')} + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{d_{S(G)}(e,e')} + \sum_{v\in V(E),e\in E(G)} q^{d_{S(G)}(e,v)} \\
&= \sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{2d_{T(G)}(v,v')} + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{2d_{T(G)}(e,e')} + \sum_{v\in V(E),e\in E(G)} q^{2d_{T(G)}(e,v)-1} \\
&= \left[\sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{2d_{T(G)}(v,v')-1} + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{2d_{T(G)}(e,e')-1} + \sum_{v\in V(E),e\in E(G)} q^{2d_{T(G)}(e,v)-1}\right] \\
&\quad + \sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{2d_{G}(v,v')}\left(1-\frac{1}{q}\right) + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{2d_{L(G)}(e,e')-1}\left(1-\frac{1}{q}\right) \\
&= \frac{1}{q}\,\mathcal{W}(T(G);q^2) + \left(1-\frac{1}{q}\right)\left[\mathcal{W}(G;q^2)+\mathcal{W}(L(G);q^2)\right]
\end{aligned}
$$

□

Other similar formulas exist:

Theorem 6 *For a connected graph G, we have*

$$
\begin{aligned}
\mathcal{W}(R(G);q) &= \mathcal{W}(T(G);q) + (q-1)\mathcal{W}(L(G);q), &(2)\\
\mathcal{W}(Q(G);q) &= \mathcal{W}(T(G);q) + (q-1)\mathcal{W}(G;q). &(3)
\end{aligned}
$$

Proof. We prove the first equation (the last equality using $d_{L(G)}(e,e') = d_{T(G)}(e,e')$) thus:

$$
\begin{aligned}
\mathcal{W}(R(G);q) &= \sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{d_{R(G)}(v,v')} + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{d_{R(G)}(e,e')} + \sum_{v\in V(E),e\in E(G)} q^{d_{R(G)}(e,v)} \\
&= \sum_{\{v,v'\}\in\binom{V(G)}{2}} q^{d_{T(G)}(v,v')} + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{d_{T(G)}(e,e')+1} + \sum_{v\in V(E),e\in E(G)} q^{d_{T(G)}(e,v)} \\
&= \mathcal{W}(T(G);q) + \sum_{\{e,e'\}\in\binom{E(G)}{2}} q^{d_{T(G)}(e,e')}(q-1) \\
&= \mathcal{W}(T(G);q) + (q-1)\mathcal{W}(L(G);q).
\end{aligned}
$$

Eq. 3 is similarly proved using the fact that $d_G(v,v') = d_{T(G)}(v,v')$. □

Remark: If we differentiate the formulas in the last two theorems with respect to q and substitute $q = 1$, then we can obtain Theorem 4. Eq. 1–3 can also be combined into

$$
\mathcal{W}(R(G);q) + \mathcal{W}(Q(G);q) - q\,\mathcal{W}(S(G);q) = 2\mathcal{W}(T(G);q) - \mathcal{W}(T(G);q^2). \qquad (4)
$$

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