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The behavior of Wiener indices and polynomials of graphs under five graph decorations

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Abstract

The sum of distances between all vertex pairs in a connected graph is known as the Wiener index. It is an early index which 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.

Mathematicians have studied several operators on a connected graph in which we see a subdivision of the edges. In this work, 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. Introducing the Wiener index and subdivision-related graphs

We first 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, [5,8,9,11]). These are called "topological indices". One index that was used very early was that of Harold Wiener, defined in 1947 [13].

Definition 1. The Wiener polynomial and Wiener index [7,13,15] of a connected graph G are

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

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 of Fig. 1(a).

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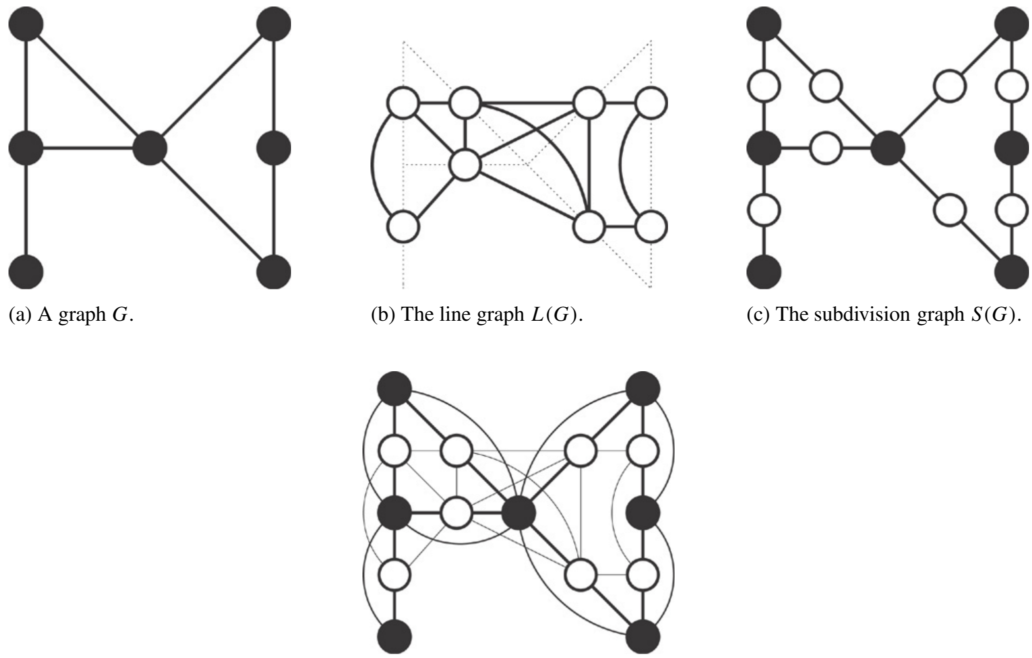


(a) A graph G.

(b) The line graph $L(G)$.

(c) The subdivision graph $S(G)$.

(d) The total graph $T(G)$.

Fig. 1. A graph G and subdivision-related graphs $L(G)$, $S(G)$ and $T(G)$.

The Wiener polynomial was first defined by Haruo Hosoya [7] with this name, in honor of Harold Wiener who first studied the index. Today the polynomial appears in slightly different forms in the literature, often as the *Hosoya polynomial*. Readers interested in the continuing saga of Wiener indices and polynomials should refer to a dedicated survey (see, e.g., [1,2,4,6,7,10,12,14,15]). In particular, the paper by Dobrynin et al. contains several of the results referred to below.

Suppose $G = (V, E)$ is a connected graph with the vertex set V and the edge set E. Given an edge $e = \{u, v\}$ of G, let $V(e)$ denote the set of two end vertices of e. Now we can define three related graphs – the *line graph* $L(G)$, the *subdivision graph* $S(G)$, the *total graph* $T(G)$ – as follows (cf. e.g., [3]):

Line graph: The vertices of $L(G)$ are the edges of G. Two edges of G that share a vertex are considered to be adjacent in $L(G)$ (see Fig. 1(b)).

Subdivision graph: $S(G)$ is the graph obtained by inserting an additional vertex in each edge of G (see Fig. 1(c)). Equivalently, each edge of G is replaced by a path of length 2.

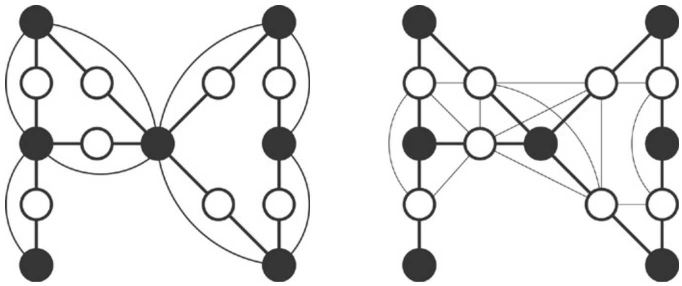
Total graph: $T(G)$ has as its vertices the edges and vertices of G. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G (see Fig. 1(d)).

Two extra subdivision-related graphs named $R(G)$ and $Q(G)$ are defined by [3]. We follow the notation of their creators, who did not see fit to give names to these graphs.

- $R(G)$ is obtained from G by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge (see Fig. 2(a)).
  Another way to describe $R(G)$ is to replace each edge of G by a triangle.
- $Q(G)$ is obtained from G by inserting a new vertex into each edge of G, then joining with edges those pairs of new vertices on adjacent edges of G (see Fig. 2(b)).

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

$$EE(G) := \left\{\{e, e'\} : e, e' \in E(G), |V(e) \cap V(e')| = 1\right\}.$$
$$EV(G) := \{\{e, v\} : V(G) \ni v \in V(e), e \in E(G)\}.$$



(a) The graph $R(G)$. (b) The graph $Q(G)$.

Fig. 2. The two additional subdivision-related graphs $R(G)$ and $Q(G)$.

We may then write the subdivision-related graphs 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 [1] 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 may be the first result to consider the relations between the Wiener indices of a graph before and after a graph operation. In Section 2 we outline our results on Wiener indices of these subdivision-related graphs, and proceed to prove them, and then in Section 3 move on the Wiener polynomials.

2. Distances in subdivision-related 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 $e \overset{e \cap e'}{\rightarrow} e'$. In other words, if $e = \{v, v'\}$ and $e' = \{v, v''\}$, then we will write $e \overset{v}{\rightarrow} e'$ 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 a shortest path (of length k) in G from v to v' be represented by the sequence

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

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 $u \overset{p}{\rightarrow} u'$. In the former, the segment of a path that proceeds along

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

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

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

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 visit 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 in $Q(G)$!). 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 $Q(G)$ 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 a shortest 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 a 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 corresponding 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 $S(G)$ is

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

Arguments similar to point 3 of Lemma 1 show that the corresponding 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 that the corresponding 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 a shortest path in $T(G)$ can be either of the above. □

Almost immediately we can prove some interesting relationships between various subdivision-related graphs:

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

$$\mathcal{W}(S(G)) = 2\mathcal{W}(T(G)) - mn;$$
$$\mathcal{W}(R(G)) = \mathcal{W}(T(G)) + m(m-1)/2;$$
$$\mathcal{W}(Q(G)) = \mathcal{W}(T(G)) + n(n-1)/2.$$

Proof. Split the sum over 2-subsets $\{x, x'\}$ of $E(G) \cup V(G)$ in 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. $\square$

Corollary 4.1. *Let G be a connected graphs with m edges and n vertices. Then*

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

We may further note [4] that if G is a tree, the Wiener index of its subdivision graph is

$$\mathcal{W}(S(G)) = 8\mathcal{W}(G) - 2n(n-1).$$

So the Wiener indices after the remaining subdivision-related graphs can be derived in short order:

Corollary 4.2. *For a tree G with n vertices,*

$$\mathcal{W}(T(G)) = 4\mathcal{W}(G) - n(n-1)/2;$$
$$\mathcal{W}(R(G)) = 4\mathcal{W}(G) - n + 1;$$
$$\mathcal{W}(Q(G)) = 4\mathcal{W}(G).$$

3. Wiener polynomials of subdivision-related graphs

We may observe that there are other ways we can use the lemmas in the above section. For example, we may derive connections between Wiener (Hosoya) polynomials of subdivision-related graphs:

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

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

Proof.

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

Other similar formulas exist:

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

$$\mathcal{W}(R(G);q) = \mathcal{W}(T(G);q) + (q-1)\mathcal{W}(L(G);q), \tag{2}$$

$$\mathcal{W}(Q(G);q) = \mathcal{W}(T(G);q) + (q-1)\mathcal{W}(G;q). \tag{3}$$

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 by using the fact that $d_G(v,v') = d_{T(G)}(v,v')$. □

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

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

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References

[1] F. Buckley, Mean distance in line graphs, Congr. Numer. 32 (1981) 153–162.
[2] F. Buckley, H. Harary, Distances in Graphs, Addison-Wesley, New York, 1990.
[3] D.M. Cvetkocić, M. Doob, H. Sachs, Spectra of Graphs—Theory and Application, Academic Press, New York, 1980.
[4] A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.
[5] I. Gutman, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089.
[6] I. Gutman, P. Hansen, H. Melot, Variable neighborhood search for extremal graphs. 10. Comparison of irregularity indices for chemical trees, J. Chem. Inf. Model. 45 (2) (2005) 222–230.
[7] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Jpn. 4 (1971) 2332–2339.
[8] D.J. Klein, D. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: A relation with the Wiener index, J. Chem. Inf. Comput. Sci. 32 (1992) 304–305.
[9] B. Mohar, D. Babić, N. Trinajstić, A novel definition of the Wiener index for trees, J. Chem. Inf. Comput. Sci. 33 (1993) 153–154.
[10] M. Randić, A.T. Balaban, S.C. Basak, On structural interpretation of several distance related topological indices, J. Chem. Inf. Comput. Sci. 41 (3) (2001) 593–601.
[11] M. Randić, J. Zupan, On interpretation of well-known topological indices, J. Chem. Inf. Comput. Sci. 41 (2001) 550–560.
[12] B. Sagan, Y.-N. Yeh, P. Zhang, The Wiener polynomial of a graph, Intern. J. Quant. Chem. 60 (1996) 959–969.
[13] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.
[14] W.G. Yan, Y.-N. Yeh, Connections between Wiener index and matchings, J. Math. Chem. 39 (2) (2006) 389–399.
[15] B.Y. Yang, Y.-N. Yeh, About Wiener Numbers and Polynomials, in: Y. Fong, et al. (Eds.), Proc. of Second International Taiwan–Moscow Algebra Workshop, Tainan, 1997, Springer, Hong Kong, 2000, pp. 203–226.