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ON THE WIENER INDEX AND LAPLACIAN COEFFICIENTS OF GRAPHS WITH GIVEN DIAMETER OR RADIUS *

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Abstract

Let G be a simple undirected n-vertex graph with the characteristic polynomial of its Laplacian matrix $L(G)$, $\det(\lambda I - L(G)) = \sum_{k=0}^{n}(-1)^k c_k \lambda^{n-k}$. It is well known that for trees the Laplacian coefficient c_{n-2} is equal to the Wiener index of G. Using a result of Zhou and Gutman on the relation between the Laplacian coefficients and the matching numbers in subdivided bipartite graphs, we characterize first the trees with given diameter and then the connected graphs with given radius which simultaneously minimize all Laplacian coefficients. This approach generalizes recent results of Liu and Pan [MATCH Commun. Math. Comput. Chem. 60 (2008), 85–94] and Wang and Guo [MATCH Commun. Math. Comput. Chem. 60 (2008), 609–622] who characterized n-vertex trees with fixed diameter d which minimize the Wiener index. In conclusion, we illustrate on examples with Wiener and modified hyper-Wiener index that the opposite problem of simultaneously maximizing all Laplacian coefficients has no solution.

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1 Introduction

Let $G = (V, E)$ be a simple undirected graph with $n = |V|$ vertices. The Laplacian polynomial $P(G, \lambda)$ of G is the characteristic polynomial of its Laplacian matrix $L(G) = D(G) - A(G)$,

$$P(G, \lambda) = \det(\lambda I_n - L(G)) = \sum_{k=0}^{n} (-1)^k c_k \lambda^{n-k}.$$

The Laplacian matrix $L(G)$ has non-negative eigenvalues $\mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_{n-1} \geqslant \mu_n = 0$ [2]. From Viette's formulas, $c_k = \sigma_k(\mu_1, \mu_2, \ldots, \mu_{n-1})$ is a symmetric polynomial of order $n-1$. In particular, $c_0 = 1$, $c_1 = 2n$, $c_n = 0$ and $c_{n-1} = n\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of G. If G is a tree, coefficient c_{n-2} is equal to its Wiener index, which is a sum of distances between all pairs of vertices.

Let $m_k(G)$ be the number of matchings of G containing exactly k independent edges. The subdivision graph $S(G)$ of G is obtained by inserting a new vertex of degree two on each edge of G. Zhou and Gutman [17] proved that for every acyclic graph T with n vertices

$$c_k(T) = m_k(S(T)), \quad 0 \leqslant k \leqslant n. \tag{1}$$

Let $C(a_1, \ldots, a_{d-1})$ be a caterpillar obtained from a path P_d with vertices $\{v_0, v_1, \ldots, v_d\}$ by attaching a_i pendent edges to vertex v_i, $i = 1, \ldots, d-1$. Clearly, $C(a_1, \ldots, a_{d-1})$ has diameter d and $n = d + 1 + \sum_{i=1}^{d-1} a_i$. For simplicity, $C_{n,d} = C(0, \ldots, 0, a_{\lfloor d/2 \rfloor}, 0, \ldots, 0)$.

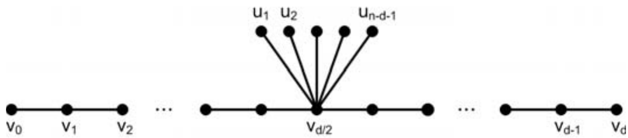

Figure 1: *Caterpillar* $C_{n,d}$.

In [12] it is shown that caterpillar $C_{n,d}$ has minimal spectral radius (the greatest eigenvalue of adjacency matrix) among graphs with fixed diameter.

Our goal here is to characterize the trees with given diameter and the connected graphs with given radius which simultaneously minimize all Laplacian coefficients. We generalize recent results of Liu and Pan [10], and Wang and Guo [15] who proved that the caterpillar $C_{n,d}$ is the unique tree with n vertices and diameter d, that minimizes Wiener index. We also deal with connected n-vertex graphs with fixed diameter, and prove that $C_{n,2r-1}$ is extremal graph.

After a few preliminary results in Section 2, we prove in Section 3 that a caterpillar $C_{n,d}$ minimizes all Laplacian coefficients among n-vertex trees with diameter d. In particular, $C_{n,d}$ minimizes the Wiener index and the modified hyper-Wiener index among such trees. Further, in Section 4 we prove that $C_{n,2r-1}$ minimizes all Laplacian coefficients among connected n-vertex graphs with radius r. Finally, in conclusion we illustrate on examples with Wiener and modified hyper-Wiener index that the opposite problem of simultaneously maximizing all Laplacian coefficients has no solution.

2 Preliminaries

The distance $d(u, v)$ between two vertices u and v in a connected graph G is the length of a shortest path between them. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex.

Definition 2.1 *The diameter $d(G)$ of a graph G is the maximum eccentricity over all vertices in a graph, and the radius $r(G)$ is the minimum eccentricity over all $v \in V(G)$.*

Vertices of minimum eccentricity form the center (see [4]). A tree T has exactly one or two adjacent center vertices. For a tree T,

$$d(T) = \begin{cases} 2r(T) - 1 & \text{if } T \text{ is bicentral,} \\ 2r(T) & \text{if } T \text{ has unique center vertex.} \end{cases} \tag{2}$$

The next lemma counts the number of matchings in a path P_n.

Lemma 2.1 *For $0 \leqslant k \leqslant \lceil \frac{n}{2} \rceil$, the number of matchings with k edges for path P_n is*

$$m_k(P_n) = \binom{n-k}{k}.$$

Proof: If v is a pendent vertex of a graph G, adjacent to u, then for the matching number of G the recurrence relation holds

$$m_k(G) = m_k(G - v) + m_{k-1}(G - u - v).$$

If G is a path, then $m_k(P_n) = m_k(P_{n-1}) + m_{k-1}(P_{n-2})$. For base cases $k = 0$ and $k = 1$ we have $m_0(P_n) = 1$ and $m_1(P_n) = n - 1$. After substituting formula for $m_k(P_n)$, we get the well-known identity for binomial coefficients.

$$\binom{n-k}{k} = \binom{n-1-k}{k} + \binom{n-2-(k-1)}{k-1}.$$

Maximum cardinality of a matching in the path P_n is $\lceil \frac{n}{2} \rceil$ and thus, $0 \leqslant k \leqslant \lceil \frac{n}{2} \rceil$. □

The union $G = G_1 \cup G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph $G = (V, E)$ with $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$. If G is a union of two paths of lengths a and b, then G is disconnected and has $a + b$ vertices and $a + b - 2$ edges.

Lemma 2.2 *Let $m_k(a, b)$ be the number of k-matchings in $G = P_a \cup P_b$, where $a + b$ is fixed even number. Then, the following inequality holds*

$$m_k\left(\left\lceil \frac{a+b}{2} \right\rceil, \left\lfloor \frac{a+b}{2} \right\rfloor\right) \leqslant \ldots \leqslant m_k(a + b - 2, 2) \leqslant m_k(a + b, 0) = m_k(P_{a+b}).$$

Proof: Without loss of generality, we can assume that $a \geqslant b$. Notice that the number of vertices in every graph is equal to $a + b$. The path P_{a+b} contains as a subgraph $P_{a'} \cup P_{b'}$, where $a' + b' = a + b$ and $a' \geqslant b' > 0$. This means that the number of k-matchings of P_{a+b} is greater than or equal to the number of k matchings of $P_{a'} \cup P_{b'}$, and therefore $m_k(a + b, 0) \geqslant m_k(a', b')$. In the sequel, we exclude P_{a+b} from consideration.

For the case $k = 0$, by definition we have identity $m_0(G) = 1$. For $k = 1$ we have equality, because

$$m_1(a', b') = (a' - 1) + (b' - 1) = a' + b' - 2 = a + b - 2.$$

We will use mathematical induction on the sum $a + b$. The base cases $a + b = 2, 4, 6$ are trivial for consideration using previous lemma. Suppose now that $a + b$ is an even number greater than 6 and consider graphs $G = P_a \cup P_b$ and $G' = P_{a'} \cup P_{b'}$, such that $a > b$ and $a' = a - 2$ and $b' = b + 2$. We divide the set of k-matchings of G' in two disjoint subsets $\mathcal{M}'_1$ and $\mathcal{M}'_2$. The set $\mathcal{M}'_1$ contains all k-matchings for which the last edge of $P_{a'}$ and the first edge of $P_{b'}$ are not together in the matching, while $\mathcal{M}'_2$ consists of k-matchings that contain both the last edge of $P_{a'}$ and the first edge of $P_{b'}$. Analogously for the graph G, we define the partition $\mathcal{M}_1 \cup \mathcal{M}_2$ of the set of k-matchings.

Consider an arbitrary matching M' from $\mathcal{M}'_1$ with k disjoint edges. We can construct corresponding matching M in the graph G in the following way: join paths $P_{a'}$ and $P_{b'}$ and form a path P_{a+b-1} by identifying the last vertex on path $P_{a'}$ and the first vertex on path $P_{b'}$. This way we get a k-matching in path $P_{a+b-1} = v_1 v_2 \ldots v_{a+b-1}$. Next, split graph P_{a+b-1} in two parts to get $P_a = v_1 v_2 \ldots v_a$ and $P_b = v_a v_{a+1} \ldots v_{a+b-1}$. Note that the last edge in P_a and the first edge in P_b are not both in the matching M. This way we establish a bijection between sets $\mathcal{M}_1$ and $\mathcal{M}'_1$.

Now consider a matching M' of G' such that the last edge of $P_{a'}$ and the first edge of $P_{b'}$ are in M'. The cardinality of the set $\mathcal{M}'_2$ equals to $m_{k-1}(a' - 2, b' - 2)$, because we cannot include the first two vertices from $P_{a'}$ and the last two vertices from $P_{b'}$ in the matching. Analogously, we conclude that $|\mathcal{M}_2| = m_{k-1}(a - 2, b - 2)$. This way we reduce problem to pairs $(a' - 2, b' - 2)$ and $(a - 2, b - 2)$ with smaller sum and inequality

$$m_{k-1}(a - 2, b - 2) \geqslant m_{k-1}(a' - 2, b' - 2)$$

holds by induction hypothesis. If one of numbers in the set $\{a, b, a', b'\}$ becomes equal to 0 using above transformation, it must the smallest number b. In that case, we have $m_{k-1}(a-2, 0) \geqslant m_{k-1}(a'-2, b'-2)$ which is already considered. $\square$

Lemma 2.3 *For every* $2 \leqslant r \leqslant \lfloor \frac{n}{2} \rfloor$, *it holds*

$$c_k(C_{n,2r}) \geqslant c_k(C_{n,2r-1}).$$

Proof: Coefficients c_0 and c_n are constant, while trees $C_{n,2r}$ and $C_{n,2r-1}$ have equal number of vertices and thus, we have equalities

$$c_1(C_{n,2r}) = c_1(C_{n,2r-1}) = 2n \quad \text{and} \quad c_{n-1}(C_{n,2r}) = c_{n-1}(C_{n,2r-1}) = n.$$

Assume that $2 \leqslant k \leqslant n - 2$. Using identity (1), we will establish injection from the set of k-matchings of subdivision graph $S(C_{n,2r-1})$ to $S(C_{n,2r})$. Let $v_0, v_1, \ldots, v_{2r-1}$ be the vertices on the main path of caterpillar $C_{n,2r-1}$ and $u_1, u_2, \ldots, u_{n-2r}$ pendent vertices from central vertex v_r. We obtain graph $C_{n,2r}$ by removing the edge $v_r u_{n-2r}$ and adding the edge $v_{2r-1} u_{n-2r}$. Assume that vertices $w_1, w_2, \ldots, w_{n-2r}$ are subdivision vertices of degree 2 on edges $v_r u_1, v_r u_2, \ldots, v_r u_{n-2r}$.

Consider an arbitrary matching M of subdivision graph $S(C_{n,2r-1})$. If M does not contain the edge $v_r w_{n-2r}$ then the corresponding set of edges in $S(C_{n,2r})$ is also a k-matching. Now assume that matching M contains the edge $v_r w_{n-2r}$. If we exclude this edge from the graph $S(C_{n,2r-1})$, we get graph $G' = S(C_{n,2r-1}) - v_r w_{n-2r} = P_{2r} \cup P_{2r-2} \cup (n-2r-1)P_2 \cup P_1$. Therefore, the number of k-matchings that contain an edge $v_r w_{n-2r}$ in $S(C_{n,2r-1})$ is equal to the number of matchings with $k-1$ edges in graph G' that is union of paths P_{2r} and $P_{2(r-1)}$ and $n-2r-1$ disjoint edges $u_1w_1, u_2w_2, \ldots,$ $u_{n-2r-1}w_{n-2r-1}$

$$\mathcal{S}' = m_{k-1}(G') = m_{k-1}(P_{2r} \cup P_{2(r-1)} \cup (n-2r-1)P_2).$$

On the other side, let G be the graph $S(C_{n,2r}) - v_{2r-1}w_{n-2r}$. Since G contains as a subgraph $P_{2(2r-1)} \cup (n-2r-1)P_2$, the number of k-matchings that contain the edge $v_{2r-1}w_{n-2r}$ is greater than or equal to the number of $(k-1)$-matchings in the union of path $P_{2(2r-1)}$ and $n-2r-1$ disjoint edges. Therefore,

$$\mathcal{S} = m_{k-1}(G) \geqslant m_{k-1}(P_{2(2r-1)} \cup (n-2r-1)P_2).$$

Path $P_{2(2r-1)}$ is obtained by adding an edge that connects the last vertex of P_{2r} and the first vertex of $P_{2(r-1)}$, and thus we get inequality

$$m_k(S(C_{n,2r})) \geqslant m_k(S(C_{n,2r-1})).$$

Finally we get that all coefficients of Laplacian polynomial of $C_{n,2r}$ are greater than or equal to those of $C_{n,2r-1}$. $\square$

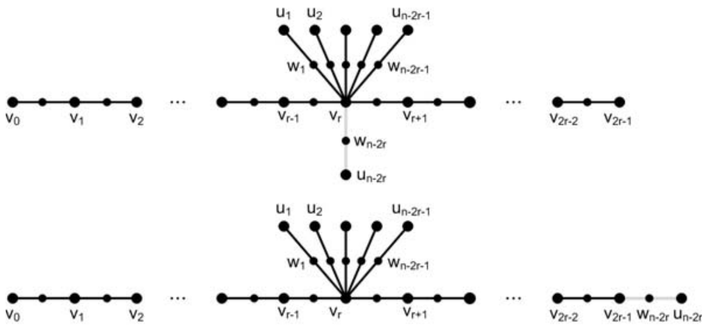

Figure 2: *Correspondence between caterpillars $C_{n,2r-1}$ and $C_{n,2r}$.*

The Laplacian coefficient c_{n-2} of a tree T is equal to the sum of all distances between unordered pairs of vertices, also known as the Wiener index,

$$c_{n-2}(T) = W(T) = \sum_{u,v \in V} d(u,v).$$

The Wiener index s considered as one of the most used topological index with high correlation with many physical and chemical indices of molecular compounds. For recent surveys on Wiener index see [4], [5], [6]. The hyper-Wiener index $WW(G)$ [7] is one of the recently introduced distance based molecular descriptors. It was proved in [8] that a modification of the hyper-Wiener index, denoted as $WWW(G)$, has certain advantages over the original $WW(G)$. The modified hyper-Wiener index is equal to the coefficient c_{n-3} of Laplacian characteristic polynomial.

Proposition 2.4 *The Wiener index of caterpillar $C_{n,d}$ equals:*

$$W(C_{n,d}) = \begin{cases} \frac{d(d+1)(d+2)}{6} + (n-d-1)(n-1) + (n-d-1)\left(\frac{d}{2}+1\right)\frac{d}{2}, & \text{if } d \text{ is even,} \\ \frac{d(d+1)(d+2)}{6} + (n-d-1)(n-1) + (n-d-1)\left(\frac{d+1}{2}\right)^2, & \text{if } d \text{ is odd.} \end{cases}$$

Proof: By summing all distances of vertices on the main path of length d, we get

$$\sum_{i=1}^{d} i(d+1-i) = (d+1)\cdot\sum_{i=1}^{d} i - \sum_{i=1}^{d} i^2 = \frac{d(d+1)(d+2)}{6}.$$

For every pendent vertex attached to $v_{\lfloor d/2 \rfloor} = v_c$ we have the same contribution in summation for the Wiener index:

$$(n-d-2) + \left(\sum_{i=0}^{d} |i-c| + 1\right) = (n-1) + \sum_{i=0}^{d} |i-c|.$$

Therefore, based on parity of d we easily get given formula. $\square$

3 Trees with fixed diameter

We need the following definition of σ-transformation, suggested by Mohar in [11].

Definition 3.1 *Let u_0 be a vertex of a tree T of degree $p+1$. Suppose that $u_0u_1, u_0u_2, \ldots, u_0u_p$ are pendant edges incident with u_0, and that v_0 is the neighbor of u_0 distinct from $u_1, u_2, \ldots, u_p$. Then we form a tree $T' = \sigma(T, u_0)$ by removing the edges $u_0u_1, u_0u_1, \ldots, u_0u_p$ from T and adding p new pendant edges $v_0v_1, v_0v_2, \ldots, v_0v_p$ incident with v_0. We say that T' is a σ-transform of T.*

Mohar proved that every tree can be transformed into a star by a sequence of σ-transformations.

Theorem 3.1 ([11]) *Let $T' = \sigma(T, u_0)$ be a σ-transform of a tree T of order n. For $d = 2, 3, \ldots k$, let n_d be the number of vertices in $T - u_0$ that are at distance d from u_0 in T. Then*

$$c_k(T) \geqslant c_k(T') + \sum_{d=2}^{k} n_d \cdot p \cdot \binom{n-2-d}{k-d} \qquad \text{for } 2 \leqslant k \leqslant n-2$$

and $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$.

Theorem 3.2 *Among connected acyclic graphs on n vertices and diameter d, caterpillar*

$$C_{n,d} = C(0, \ldots, 0, a_{\lfloor d/2 \rfloor}, 0, \ldots, 0),$$

where $a_{\lfloor d/2 \rfloor} = n-d-1$, has minimal Laplacian coefficient c_k, for every $k = 0, 1, \ldots, n$.

Proof: Coefficients c_0, c_1, c_{n-1} and c_n are constant for all trees on n vertices. The star graph S_n is the unique tree with diameter 2 and path P_n is unique graph with diameter $n-1$. Therefore, we can assume that $2 \leqslant k \leqslant n-2$ and $3 \leqslant d \leqslant n-2$.

Let $P = v_0v_1v_2 \dots v_d$ be a path in tree T of maximal length. Every vertex v_i on the path P is a root of a tree T_i with $a_i + 1$ vertices, that does not contain other vertices of P. We apply σ-transformation on trees $T_1, T_2, \dots, T_{d-1}$ to decrease coefficients c_k, as long as we do not get a caterpillar $C(a_0, a_1, a_2, \dots, a_d)$. By a theorem of Zhou and Gutman, it suffices to see that

$$m_k(S(C(a_1, a_2, \dots, a_{d-1}))) > m_k(S(C_{n,d})).$$

Assume that $v_{\lfloor d/2 \rfloor} = v_c$ is a central vertex of $C_{n,d}$. Let $u_1, u_2, \dots, u_{n-d-1}$ be pendent vertices attached to v_c in $S(C_{n,d})$, and let $w_1, w_2, \dots, w_{n-d-1}$ be subdivision vertices on pendent edges $v_cu_1, v_cu_2, \dots, v_cu_{n-d-1}$. We also introduce ordering of pendent vertices. Namely, in the graph $C_n(a_1, a_2, \dots, a_{d-1})$ first a_1 vertices in the set $\{u_1, u_2, \dots, u_{n-d-1}\}$ are attached to v_1, next a_2 vertices are attached to v_2, and so on.

Consider an arbitrary matching M' with k edges in caterpillar $S(C_{n,d})$. If M does not contain any of the edges $\{v_cw_1, v_cw_2, \dots, v_cw_{n-d-1}\}$, then we can a construct matching in $S(C(a_1, a_2, \dots, a_{d-1}))$, by taking corresponding edges from M. If the edge v_cw_i is in the matching M' for some $1 \leqslant i \leqslant n-d-1$, the corresponding edge v_jw_i is attached to some vertex v_j, where $1 \leqslant j \leqslant d-1$. Moreover, if we fix the number l of matching edges in the set

$$\{u_1w_1, u_2w_2, \dots, u_{i-1}w_{i-1}, u_{i+1}w_{i+1}, \dots, u_{n-d-1}w_{n-d-1}\},$$

we have to choose exactly $k - l - 1$ independent edges in the remaining graphs. Caterpillar $S(C_{n,d})$ is decomposed into two path of lengths $2\lfloor \frac{d}{2} \rfloor$ and $2\lceil \frac{d}{2} \rceil$, and caterpillar $S(C(a_1, a_2, \dots, a_{d-1}))$ is decomposed in paths of lengths $2j$ and $2d - 2j$. From Lemma 2.2 we can see that

$$m_{k-l-1}(2\left\lfloor \frac{d}{2} \right\rfloor, 2\left\lceil \frac{d}{2} \right\rceil) \leqslant m_{k-l-1}(2j, 2d-2j).$$

If we sum this inequality for $l = 0, 1, \dots, k-1$, we obtain that the number of k-matchings in graph $S(C_{n,d})$ is less than the number of k-matchings in $S(C(a_0, a_1, a_2, \dots, a_d))$. Thus, for every tree T on n vertices with diameter d holds:

$$c_k(C_{n,d}) \leqslant c_k(T), \quad k = 0, 1, 2, \dots n.$$

$\square$

4 Graphs with fixed radius

Theorem 4.1 *Among connected graphs on n vertices and radius r, caterpillar $C_{n,2r-1}$ has minimal coefficient c_k, for every $k = 0, 1, \dots, n$.*

Proof: Let v be a center vertex of G and let T be a spanning tree of G with shortest paths from v to all other vertices. Tree T has radius r and can be obtained by performing the breadth first search algorithm (see [3]). Laplacian eigenvalues of an edge-deleted graph $G - e$ interlace those of G,

$$\mu_1(G) \geqslant \mu_1(G-e) \geqslant \mu_2(G) \geqslant \mu_2(G-e) \geqslant \dots \geqslant \mu_{n-1}(G) \geqslant \mu_{n-1}(G-e) \geqslant 0.$$

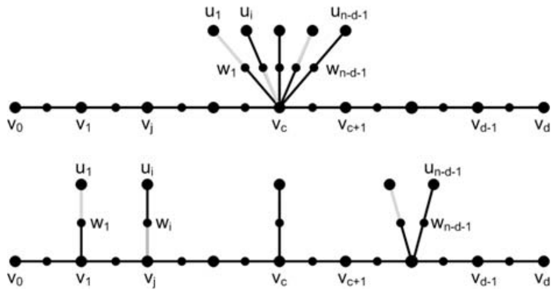

Figure 3: *Correspodence between caterpillars $C_{n,d}$ and $C(a_0, a_1, \dots, a_d)$.*

Since, $c_k(G)$ is equal to k-th symmetric polynomial of eigenvalues $(\mu_1(G), \mu_2(G), \dots, \mu_{n-1}(G))$, we have $c_k(G) \geqslant c_k(G-e)$. Thus, we delete edges of G until we get a tree T with radius r. This way we do not increase Laplacian coefficients c_k. The diameter of tree T is either $2r-1$ or $2r$. Since $c_k(C_{n,2r-1}) \leqslant c_k(C_{n,2r})$ from Lemma 2.3 we conclude that extremal graph on n vertices, which has minimal coefficients c_k for fixed radius r, is the caterpillar $C_{n,2r-1}$. □

We can establish analogous result on the Wiener index.

Corollary 4.2 *Among connected graphs on n vertices and radius r, caterpillar $C_{n,2r-1}$ has minimal Wiener index.*

5 Concluding remarks

We proved that $C_{n,2r-1}$ is the unique graph that minimize all Laplacian coefficients simultaneously among graphs on n vertices with given radius r. In the class of n-vertex graphs with fixed diameter, we found the graph with minimal Laplacian coefficients in case of trees—because it is not always possible to find a spanning tree of a graph with the same diameter.

Naturally, one wants to describe n-vertex graphs with fixed radius or diameter with maximal Laplacian coefficients. We have checked all trees up to 20 vertices and classify them based on diameter and radius. For every triple (n, d, k) and (n, r, k) we found extremal graphs with n vertices and fixed diameter d or fixed radius r that maximize coefficient c_k. The result is obvious—trees that maximize Wiener index are different from those with the same parameters that maximize modified hyper-Wiener index.

The following two graphs on the Figure 4 are extremal for $n = 18$ vertices with diameter $d = 4$; the first graph is a unique tree that maximizes Wiener index $c_{n-2} = 454$ and the second one is also a unique tree that maximizes modified hyper-Wiener index $c_{n-3} = 4960$.

The following two graphs on the Figure 5 are extremal for $n = 17$ vertices with radius $r = 5$; the first graph is a unique tree that maximizes Wiener index $c_{n-2} = 664$ and the second one is also a unique tree that maximizes modified hyper-Wiener index $c_{n-3} = 9173$.

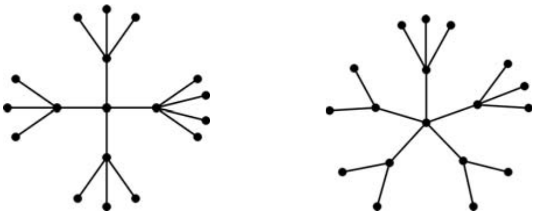

Figure 4: *Graphs with $n = 18$ and $d = 4$ that maximize c_{16} and c_{15}.*

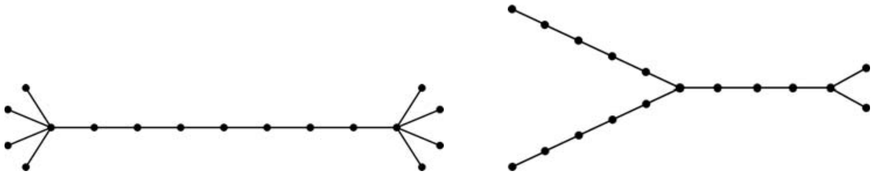

Figure 5: *Graphs with $n = 17$ and $r = 5$ that maximize c_{15} and c_{14}.*

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