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On Graphs with Same Distance Distribution

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Abstract

In the present paper we investigate the relationship between Wiener number W, hyper-Wiener number R, Wiener vectors WV, hyper-Wiener vectors HWV, Wiener polynomial H, hyper-Wiener polynomial HH and distance distribution DD of a (molecular) graph. It is shown that for connected graphs G and G^*, the following five statements are equivalent: 1) $DD(G) = DD(G^*)$, 2) $WV(G) = WV(G^*)$, 3) $HWV(G) = HWV(G^*)$, 4) $H(G) = H(G^*)$, 5) $HH(G) = HH(G^*)$; and if G and G^* have same distance distribution DD then they have same W and R but the contrary is not true. Therefore, we further investigate the graphs with same distance distribution. Some construction methods for finding graphs with same distance distribution are given.

Keywords

Distance Distribution, Distance Matrix, Wiener Vector, Hyper-Wiener Vector

1. Introduction

The Wiener index is one of the oldest topological indices of molecular structures. It was put forward by the physico-chemist Harold Wiener [1] in 1947. The Wiener index of a connected graph G is defined as the sum of distances between all pairs of vertices in G:

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

where $V(G)$ is the vertex set of G, and $d_G(u,v)$ is the distance between vertices u and v in G.

As an extension of the Wiener index of a tree, Randić [2] introduced Wiener matrix $\mathbf{W}$ and hyper-Wiener index R of a tree. 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 $T_{2,\pi(i,j)}$, respectively. Then the Wiener matrix W and the hyper-Wiener number R of T can be given by $W = (w_{ij})$, $w_{ij} = n_{1,\pi(i,j)} \cdot n_{2,\pi(i,j)}$, and $R = \sum_{i<j} w_{ij}$.

In Refs. [3] [4], 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 ${}^{1}W, {}^{2}W, {}^{3}W, \cdots$, where ${}^{k}W = \sum_{d_{i,j}=k, i<j} w_{ij}$. It is not difficult to see ${}^{1}W = W$, and $R = \sum_{k=1,2,\cdots} {}^{k}W$.

After the hyper-Wiener index of a tree was introduced, many publications [5]-[11] have appeared on calculation and generalization of the hyper-Wiener index. Klein *et al.* [5] generalized the hyper-Wiener index so as to be applicable to any connected structure. Their formula for the hyper-Wiener index R of a graph G is

$$R = R(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left(d_G^2(u,v) + d_G(u,v) \right).$$

The relation between Hyper-Wiener and Wiener index was given by Gutman [11].

The Hosoya polynomial $H(G)$ of a connected graph G was introduced by Hosoya [12] in 1988, which he named as the Wiener polynomial of a graph:

$$H = H(G,x) = \sum_{k \geq 0} d(G,k) x^k,$$

where $d(G,k)$ is the number of pairs of vertices in the graph G that are distance k apart.

In Ref. [13], Cash introduced a new hyper-Hosoya polynomial

$$HH = HH(G,x) = \sum_{k \geq 0} \frac{(k+1)}{2} d(G,k) x^k.$$

The relationship between the Hosoya polynomial and the Hyper-Hosoya polynomial was discussed [13].

The sequence $(d(G,1), d(G,2), \cdots)$ is also known (since 1981) as the distance distribution of a graph G [14], denoted by $DD(G)$. It is easy to see that $W = \sum_{k \geq 0} k \cdot d(G,k)$.

Later the definition of higher Wiener numbers is extended to be applicable to any connected structure by Guo *et al.* [15]. For a connected graph G with n vertices, denoted by $1, 2, \cdots, n$, let $w_{ij,k} = \max\{d_{ij} - k + 1, 0\}$ where d_{ij} is the distance between vertices i and j. Then ${}^{k}W = \sum_{i<j} w_{ij,k}$, $k = 1, 2, \cdots$, are called the higher Wiener numbers of G. The vector $\left({}^{1}W, {}^{2}W, \cdots\right)$ is called the hyper-Wiener vector of G, denoted by $HWV(G)$. The concept of the Wiener vector of a graph is also introduced in ref. [15]. For a connected graph G with n vertices, denoted by $1, 2, \cdots, n$, let $W_k = \sum_{i<j, d(ij)=k} d_{ij}$, $k = 1, 2, \cdots$. The vector $(W_1, W_2, \cdots)$ is called the Wiener vector of G, denoted by $WV(G)$.

Moreover, a matrix sequence $\left(W^{(1)}, W^{(2)}, W^{(3)}, \cdots\right)$, called the Wiener matrix

sequence, and their sum $\sum_{k=1,2,\cdots} W^{(k)} = W^{(H)}$, called the hyper-Wiener matrix, are introduced, where $W^{(1)} = D$ is the distance matrix. A Wiener polynomial sequence and a weighted hyper Wiener polynomial of a graph are also introduced.

In this paper, based on the results in ref. [15], we study the relation between Wiener number W, hyper-Wiener number R, Wiener vector WV, hyper-Wiener vector HWV, Hosoya polynomial H, hyper-Hosoya polynomial HH and distance distribution DD of a graph. It is shown that for connected graphs G and G^*, the the contrary is not true. This means that the distance distribution of a graph is an important topological index of molecular graphs. Therefore, we further investigate the graphs with same distance distribution. It is shown that the graphs with same vertex number, edge number, and diameter 2 have same distance distribution. Some construction methods for finding graphs with same distance distribution are given.

2. The Relation between W, R, WV, HWV, H, HH, DD

Let $diam(G)$ denote the diameter of a graph G.

Theorem 2.1. Let G and G^* be connected graphs. Then the following five statements are equivalent:

1) G and G^* have same distance distribution DD;
2) G and G^* have same Wiener vector WV;
3) G and G^* have same hyper-Wiener vector HWV;
4) G and G^* have same Wiener polynomial H;
5) G and G^* have same hyper-Wiener polynomial HH.

Proof. We shall show the equivalent statements by $(1)\Rightarrow(2)\Rightarrow(3)\Rightarrow(4)\Rightarrow(5)\Rightarrow(1)$.

$(1)\Rightarrow(2)$. By the definitions of DD and WV,

$$DD(G) = \left(d(G,1), d(G,2), \cdots, d(G, diam(G))\right), \text{ and}$$

$$WV(G) = \left(W_1, W_2, \cdots, W_{diam(G)}\right) = \left(1d(G,1), 2d(G,2), \cdots, diam(G)d(G, diam(G))\right).$$

Clearly, if $DD(G) = DD(G^*)$, then $WV(G) = WV(G^*)$.

$(2)\Rightarrow(3)$. If $WV(G) = WV(G^*)$, then $W_k = \sum_{i<j, d_{ij}=k} d_{ij} = W_k^* = \sum_{i<j, d_{ij}^*=k} d_{ij}^*$ for $k = 1, 2, \cdots, diam(G)$. So
$${}^k W = \sum_{i<j} w_{ij,k} = \sum_{i<j} \max\{d_{ij} - k + 1, 0\} = \sum_{i<j} \max\{d_{ij}^* - k + 1, 0\} = \sum_{i<j} w_{ij,k}^* = {}^k W^*$$
for $k = 1, 2, \cdots, diam(G)$. Hence $HWV(G) = HWV(G^*)$.

$(3)\Rightarrow(4)$. Suppose $HWV(G) = HWV(G^*)$. Then ${}^k W = {}^k W^*$ for $k = 1, 2, \cdots,$ and $diam(G) = diam(G^*)$.

If $k = diam(G) = diam(G^*)$, then
$$\begin{aligned} {}^k W &= \sum_{i<j} \max\{d_{ij} - k + 1, 0\} = d(G, diam(G)) \\ &= {}^k W^* = \sum_{i<j} \max\{d_{ij}^* - k + 1, 0\} = d(G^*, diam(G^*)) \end{aligned}.$$

Assume, for $1 < l \le k \le diam(G)$, $d(G,k) = d(G^*, k)$. Let $k = l - 1$. Then
$$\begin{aligned} {}^{l-1} W &= \sum_{i<j} \max\{d_{ij} - l + 2, 0\} = d(G, l-1) + \sum_{i<j, d_{ij}>l-1} \max\{d_{ij} - l + 2, 0\} \\ &= d(G, l-1) + \sum_{i<j, d_{ij}=k'>l-1} d(G, k')(k' - l + 2) \end{aligned}, \text{ and}$$

$$^{l-1}W^* = \sum_{i<j} \max\left\{d_{ij}^* - l + 2, 0\right\} = d\left(G^*, l-1\right) + \sum_{i<j, d_{ij}^* > l-1} \max\left\{d_{ij}^* - l + 2, 0\right\}$$
$$= d\left(G^*, l-1\right) + \sum_{i<j, d_{ij}^* = k' > l-1} d\left(G^*, k'\right)\left(k' - l + 2\right) = {}^{l-1}W$$

By induction hypothesis,

$\sum_{i<j,\, d_{ij}=k'>l-1} d\left(G, k'\right)\left(k' - l + 2\right) = \sum_{i<j, d_{ij}^*=k'>l-1} d\left(G^*, k'\right)\left(k' - l + 2\right)$. So we have $d\left(G, l-1\right) = d\left(G^*, l-1\right)$.

Now it follows that $d\left(G, k\right) = d\left(G^*, k\right)$ for $k = 1, 2, \cdots$, and so

$$H\left(G, x\right) = \sum_{k \geq 0} d\left(G, k\right) x^k = \sum_{k \geq 0} d\left(G^*, k\right) x^k = H\left(G^*, x\right).$$

(4)$\Rightarrow$(5). By the definitions of Hosoya polynomial H and hyper-Hosoya polynomial HH, it is easy to see that, if $H\left(G, x\right) = H\left(G^*, x\right)$, then $HH\left(G, x\right) = HH\left(G^*, x\right)$.

(5)$\Rightarrow$(1). If $HH\left(G, x\right) = HH\left(G^*, x\right)$, then $d\left(G, k\right) = d\left(G^*, k\right)$ for $k = 1, 2, \cdots$. Therefore $DD(G) = DD\left(G^*\right)$. $\square$

Theorem 2.2. Let G and G^* be two graphs with same distance distribution. Then G and G^* have same W and R.

Proof: By the definitions of DD, W and R,

$$DD(G) = \left(d(G,1), d(G,2), \cdots, d(G, diam(G))\right), \quad W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G\left(u, v\right),$$

and $R(G) = \dfrac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left(d_G^2\left(u, v\right) + d_G\left(u, v\right)\right)$.

Clearly, if $DD(G) = DD\left(G^*\right)$, then $W(G) = W\left(G^*\right)$ and $R(G) = R\left(G^*\right)$. $\square$

However, the contrary of the theorem doesn't hold. For instance, the trees T_1 and T_1^* (resp. T_2 and T_2^*) in **Figure 1** have same W and R, but they have different distance distributions.

3. Graphs with Same Distance Distribution

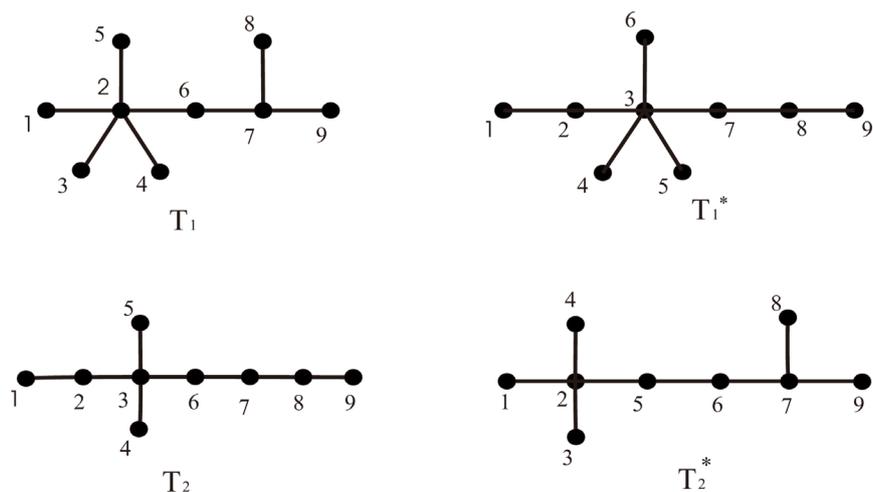From the above theorems, one can see that, if two graphs G and G^* have

Figure 1. $W(T_1) = W\left(T_1^*\right) = 86$, $R(T_1) = R\left(T_1^*\right) = 166$, $DD(T_1) = (8, 14, 6, 8)$, $DD\left(T_1^*\right) = (8, 13, 9, 5, 1)$. $W(T_2) = W\left(T_2^*\right) = 98$, $R(T_2) = R\left(T_2^*\right) = 217$, $DD(T_2) = (8, 10, 8, 5, 4, 1)$, $DD\left(T_2^*\right) = (8, 11, 6, 5, 6)$.

same distance distribution DD, then they have same W, WW, WV, HWV, H and HH. So it is significant to study the graphs with same distance dis- tribution.

1) The minimum non-isomorphic acyclic graphs with same DD

By direct calculation, we know the minimum non-isomorphic acyclic graphs with same distance distribution are the following two pairs of trees in **Figure 2** which have 9 vertices.

2) The minimum non-isomorphic cyclic graphs with same DD

The minimum non-isomorphic cyclic graphs with same distance distribution are the following graphs with 4 vertices (see **Figure 3**).

Note that, for the above graphs with same distance distribution, their Wiener matrix sequences and hyper-Wiener matrices are different.

The following theorem gives a class of graphs with same distance distribution.

Let $\mathcal{G}_{n,m}$ be the set of all the graphs with n vertices and m edges.

Theorem 3.1. Let $G, G^* \in \mathcal{G}_{n,m}$, and $diam(G) = diam(G^*) = 2$. Then $DD(G) = DD(G^*)$.

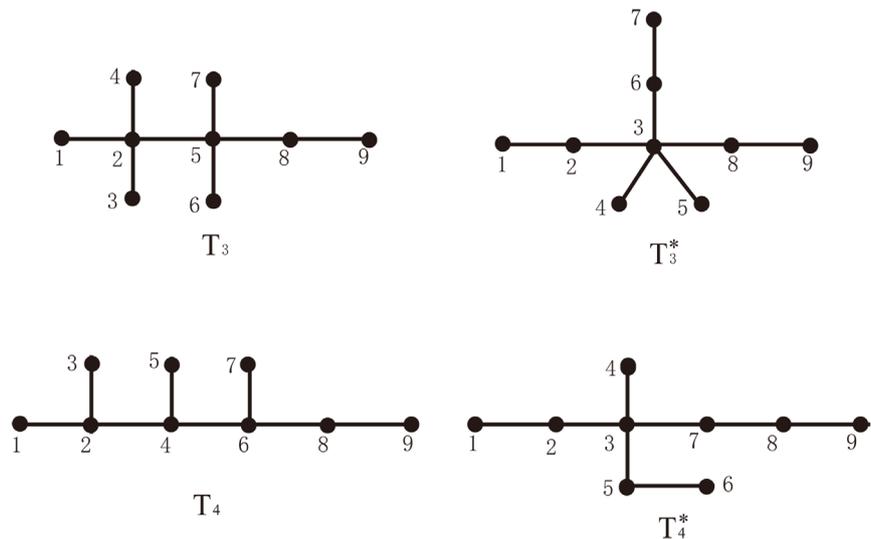**Proof.** Since $G, G^* \in \mathcal{G}_{n,m}$ and $diam(G) = diam(G^*) = 2$, we have

Figure 2. $W(T_3) = W(T_3^*) = 82$, $R(T_3) = R(T_3^*) = 149$, $DD(T_3) = DD(T_3^*) = (8,13,12,3)$. $W(T_4) = W(T_4^*) = 92$, $R(T_4) = R(T_4^*) = 188$, $DD(T_4) = DD(T_4^*) = (8,10,10,6,2)$.
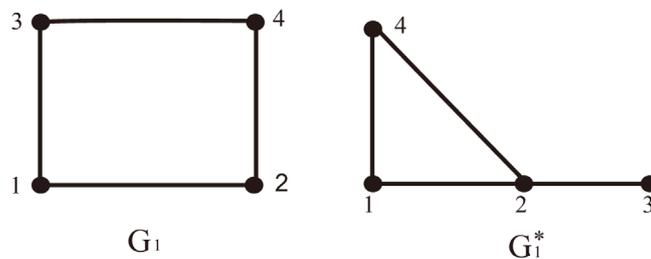

Figure 3. $W(G_1) = W(G_1^*) = 8$, $R(G_1) = R(G_1^*) = 10$, $DD(G_1) = DD(G_1^*) = (4,2)$.

$$d(G,1) = d(G^*,1) = m, \quad d(G,2) = d(G^*,2) = \binom{n}{2} - m, \quad d(G,k) = d(G^*,k) = 0$$

for $k \geq 3$, and so $DD(G) = DD(G^*)$.

Corollary 3.2. If $\binom{n}{2} > m > \binom{n}{2} - n + 1$, then all graphs in $\mathcal{G}_{n,m}$ have same distance distribution.

Proof. For $\forall G \in \mathcal{G}_{n,m}$ with $\binom{n}{2} > m > \binom{n}{2} - n + 1$, clearly $diam(G) \geq 2$.

We assert that $diam(G) = 2$.

Otherwise, there exist two vertices $u, v \in V(G)$ such that $d(u,v) \geq 3$. Let P be a shortest (u,v)-path. Then any vertex not on P is not adjacent to at least one of u and v, and the number of pairs of non-adjacent vertices on P is equal to $\big(|V(P)|-2\big) + \big(|V(P)|-3\big) + \cdots + 1 = \big(|V(P)|-2\big)\big(|V(P)|-1\big)/2$. So

$$m \leq \binom{n}{2} - \big(n - |V(P)|\big) - \big(|V(P)|-2\big)\big(|V(P)|-1\big)/2$$
$$= \binom{n}{2} - n - \big[\big(|V(P)|-2\big)\big(|V(P)|-3\big) - 4\big]/2 \leq \binom{n}{2} - n + 1$$

, contradicting that

$$m > \binom{n}{2} - n + 1.$$

Hence, by Theorem 3.1, if $m > \binom{n}{2} - n + 1$, all graphs in $\mathcal{G}_{n,m}$ have same distance distribution. $\square$

Let $G \bigvee H$ denote the graph obtained from vertex-disjoint graphs G and H by connecting every vertex of G to every vertex of H.

Corollary 3.3. Let $G_1^1, G_2^1 \in \mathcal{G}_{n_1,m_1}$ and $G_1^2, G_2^2 \in \mathcal{G}_{n_2,m_2}$. Then $G_1^1 \bigvee G_1^2$ and $G_2^1 \bigvee G_2^2$ have same distance distribution.

Proof. Obviously, $\left| V\left(G_1^1 \bigvee G_1^2 \right) \right| = \left| V\left(G_2^1 \bigvee G_2^2 \right) \right| = n_1 + n_2$, $diam\left(G_1^1 \bigvee G_1^2 \right) = diam\left(G_2^1 \bigvee G_2^2 \right) = 2$, and $\left| E\left(G_1^1 \bigvee G_1^2 \right) \right| = \left| E\left(G_2^1 \bigvee G_2^2 \right) \right| = m_1 + m_2 + n_1 \cdot n_2$. By Theorem 3.1, $DD\left(G_1^1 \bigvee G_1^2 \right) = DD\left(G_2^1 \bigvee G_2^2 \right)$.

For graphs with diameter greater than or equal to 2, we will give some construction methods for finding graphs with same distance distribution.

Let G be a connected graph with vertices set $\{v_1, v_2, \cdots, v_n\}$, and let $\mathbf{D}(G) = (d_{ij})$ be the distant matrix of the graph G. Let $d_k^G(v_i)$ denote the number of the vertices at distance k from a vertex v_i in G, and let $DD_G(v_i) = \left(d_1^G(v_i), d_2^G(v_i), \cdots, d_{diam(G)}^G(v_i) \right)$ be the distance distribution of v_i in G.

Theorem 3.4. Let G_1 and G_2 (resp. G_1' and G_2') be the connected graphs with n_1 (resp. n_2) vertices and with same distance distribution. For $v_1 \in V(G_1)$, $v_2 \in V(G_2)$, $v_1' \in V(G_1')$, and $v_2' \in V(G_2')$, let G (resp. G^*) be the graph ob-tained from G_1 and G_1' (resp. G_2 and G_2') by identifying v_1 and v_1' (resp. v_2 and v_2'). If $DD_{G_1}(v_1) = DD_{G_2}(v_2)$ and $DD_{G_1'}(v_1') = DD_{G_2'}(v_2')$, then G and G^* have same distance distribution.

Proof. It is enough to prove $d(G,k) = d(G^*,k)$ for $k = 1, 2, \cdots$.

Clearly, $d(G,k) = d(G_1,k) + d(G_1',k) + \sum_{1 \leq i,j \leq k, i+j=k} d_i^{G_1}(v_1) d_j^{G_1'}(v_1')$. Similarly, $d(G^*,k) = d(G_2,k) + d(G_2',k) + \sum_{1 \leq i,j \leq k, i+j=k} d_i^{G_2}(v_2) d_j^{G_2'}(v_2')$. Because $DD(G_1) = DD(G_2)$, $DD(G_1') = DD(G_2')$, $DD_{G_1}(v_1) = DD_{G_2}(v_2)$, $DD_{G_1'}(v_1') = DD_{G_2'}(v_2')$, we have $d(G,k) = d(G^*,k)$ for $k = 1,2,\cdots$. Hence $DD(G) = DD(G^*)$. $\square$

Theorem 3.5. Let $G_i \in \mathcal{G}_{n,m}$, $i = 1,2$, and let $S_i \subset V(G_i)$ such that any two vertices in S_i have distance less than or equal to 2 in G_i, and $|S_1| = |S_2|$. Let $G_i\{S_i\}$ denote the graph obtained from G_i by contracting vertices in S_i to a vertex s_i. Let G_i^* be the graph obtained from G_i by adding a new vertex x_i and connecting x_i to every vertex in S_i. If $DD(G_1) = DD(G_2)$ and $DD_{G_1\{S_1\}}(s_1) = DD_{G_2\{S_2\}}(s_2)$, then $DD(G_1^*) = DD(G_2^*)$.

Proof. Clearly, by the conditions of the theorem,
$$DD(G_i^*) = DD(G_i) + DD_{G_i^*}(x_i) = DD(G_i) + \left(|S_i|, 1 + d_1^{G_i\{S_i\}}(x_i), 1 + d_2^{G_i\{S_i\}}(x_i), \cdots\right),$$
$i = 1,2$. So, if $DD(G_1) = DD(G_2)$ and $DD(G_1') = DD(G_2')$ and $DD_{G_1\{S_1\}}(s_1) = DD_{G_2\{S_2\}}(s_2)$, then $DD_{G_1^*} = DD_{G_2^*}$. $\square$

From Theorem 3.4, we have the following corollary:

Corollary 3.6. Let $G_1, G_2 \in \mathcal{G}_{n,m}$ and $DD(G_1) = DD(G_2)$. Let H be a connected graph vertex-disjoint with G_1 and G_2. For $v_1 \in V(G_1)$, $v_2 \in V(G_2)$, and $u \in V(H)$, let G (resp. G^*) be the graph obtained from G_1 (resp. G_2) and H by identifying v_1 and u (resp. v_2 and u). If $DD_{G_1}(v_1) = DD_{G_2}(v_2)$, then G and G^* have same distance distribution.

From Theorem 3.5, one can obtain graphs with same distance distribution in $\mathcal{G}_{n,m}$ from graphs in $\mathcal{G}_{n-1,m-s}$ with same distance distribution by adding a new vertex and some edges.

Figure 4 shows two pairs of graphs with 5 vertices and 5 edges and with same DD, one of which has diameter 2 and the other has diameter 3.

Figure 5 shows three pairs of graphs with 6 vertices and 6 edges and with
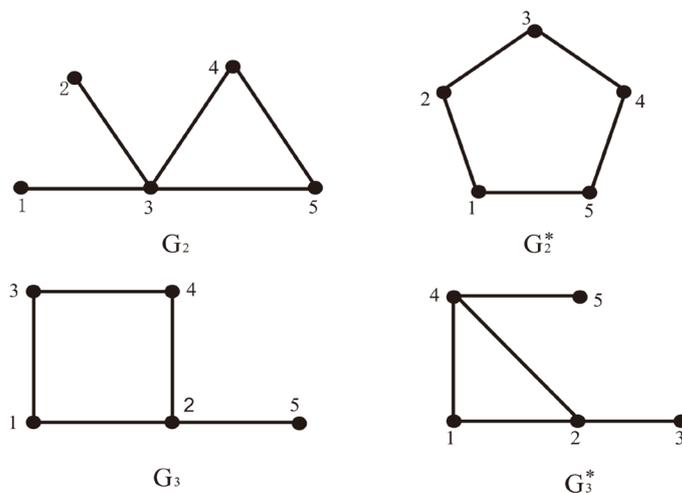

Figure 4. $W(G_2) = W(G_2^*) = 15$, $R(G_2) = R(G_2^*) = 20$, $DD(G_2) = DD(G_2^*) = (5,5)$. $W(G_3) = W(G_3^*) = 16$, $R(G_3) = R(G_3^*) = 23$, $DD(G_3) = DD(G_3^*) = (5,4,1)$.
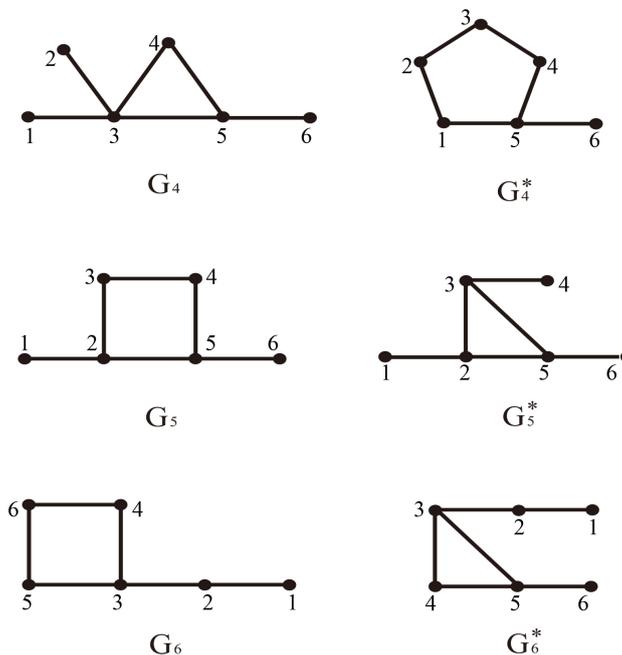
Figure 5. $W(G_4) = W(G_4^*) = 26$, $R(G_4) = R(G_4^*) = 39$, $DD(G_4) = DD(G_4^*) = (6,7,2)$. $W(G_5) = W(G_5^*) = 27$, $R(G_5) = R(G_5^*) = 42$, $DD(G_5) = DD(G_5^*) = (6,6,3)$. $W(G_6) = W(G_6^*) = 29$, $R(G_6) = R(G_6^*) = 49$, $DD(G_6) = DD(G_6^*) = (6,5,3,1)$.

same DD, two of which have diameter 3 and the other has diameter 4.

It is easy to see that the graphs in Figure 5 can be obtained from graphs in Figure 3, Figure 4 by the construction methods given in Theorems 3.4, 3.5.

However, the construction methods are not complete. There might be some graphs with same DD which could not be obtained by the above construction methods.

Open Problem. Is there a construction method for finding all graphs with same distance distribution?

Acknowledgements

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