MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 213-220

ISSN 0340 - 6253

Properties of Degree Distance and Gutman Index of Uniform Hypergraphs

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(Received October 6, 2016)

Abstract

Klein et al. found in [Molecular topological index: a relation with the Wiener index, J. Chem. Inf. Comput. Sci. 32 (1992) 304–305] a relation between degree distance and Wiener index for trees, and Gutman found in [Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089] a relation between Gutman index and Wiener index for trees. We extend these relations to uniform hypergraphs.

1 Introduction

A hypergraph G consists of a vertex set V and an edge set E, where each edge $e \in E$ is a subset of V with at least two elements. For an integer $k \geq 2$, if every edge has size k, then G is called a k-uniform hypergraph. In particular, a (simple) graph is a 2-uniform hypergraph. Hypergraph theory found applications in chemistry, see, e.g. [12, 19–21].

For distinct vertices u and v in a hypergraph G, if there is an edge containing both of them, then we say that they are adjacent, written $u \sim v$. The degree of a vertex u in G, denoted by d_u, is the number of edges of G which contain u.

For $u, v \in V$, a path from u to v of length p in G is defined to be a sequence of vertices and edges $(v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$ with all v_i distinct and all e_i distinct such that edge e_i contains vertices v_{i-1}, v_i for $i = 1, \ldots, p$, where $v_0 = u$ and $v_p = v$. A cycle of length p in G is defined to be a sequence of vertices and edges $(v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$

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with $p \geq 2$, all v_i distinct except $v_0 = v_p$ and all e_i distinct such that edge e_i contains vertices v_{i-1}, v_i for $i = 1, \ldots, p$. If there is a path from u to v for any $u, v \in V$, then G is connected.

A hypertree is a connected hypergraph with no cycle. A k-uniform hypertree with m edges always has $1 + (k-1)m$ vertices.

The distance between vertices u and v in a connected hypergraph G is the length of a shortest path from u to v in G, denoted by D_{uv}.

The Wiener index $W(G)$ of a connected hypergraph G is defined as the summation of distances between all unordered pairs of distinct vertices in G, i.e.,

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

Obviously, $W(G) = \frac{1}{2} \sum\limits_{u \in V} \sum\limits_{v \in V} D_{uv}$. The Wiener index of a connected graph has a long history [7, 13, 14, 25, 27, 28, 33]. Very recently, among others we determine in [10] the unique k-uniform hypertrees with maximum, second maximum and third maximum Wiener indices, as well as the unique k-uniform hypertrees with minimum, second minimum and third minimum Wiener indices, respectively.

The degree distance of a connected hypergraph G is defined as

$$DD(G) = \sum_{\{u,v\} \subseteq V} (d_u + d_v) D_{uv} \ .$$

Obviously, $DD(G) = \frac{1}{2} \sum\limits_{u \in V} \sum\limits_{v \in V} (d_u + d_v) D_{uv} = \sum\limits_{u \in V} d_u \sum\limits_{v \in V} D_{uv}$. For a connected graph, it was introduced by Dobrynin and Kochetova [6] and has attracted much attention, see, e.g., [1, 2, 4, 8, 11, 15, 17, 24, 32, 35]. Note that, for a graph G, the degree distance $DD(G)$ is the essential part of the molecular topological index $MTI(G)$ introduced by Schultz [29], which is defined as $MTI(G) = \sum_{u \in V} d_u^2 + DD(G)$, see also [5, 11, 16, 17, 29, 34].

The Gutman index of a connected hypergraph G is defined as

$$Gut(G) = \sum_{\{u,v\} \subseteq V} d_u d_v D_{uv} \ .$$

Obviously, $Gut(G) = \frac{1}{2} \sum\limits_{u \in V} \sum\limits_{v \in V} d_u d_v D_{uv}$. For a connected graph, it was introduced in [11] (see also [30, 31]) and has been studied extensively, see, e.g. [1, 3, 9, 18, 22, 23, 26].

For a tree G on n vertices, Klein et al. [17] (and Gutman [11]) showed that

$$DD(G) = 4W(G) - n(n-1) \, ,$$

and Gutman [11] showed that

$$Gut(G) = 4W(G) - (n-1)(2n-1)\ .$$

In this paper, we extend these two relations to hypergraphs.

2 Results

In a k-uniform hypertree G, any two edges share at most one vertex in common. This fact will be used in our proof.

Theorem 1. *Let G be a k-uniform hypertree with n vertices, where $2 \leq k \leq n$. Then*

$$(k-1)DD(G) = 2kW(G) - n(n-1).$$

Proof. Let $m = |E|$. Then $m = \frac{n-1}{k-1}$ and $\sum\limits_{u\in V} d_u = km$. Note that

$$2\sum_{\substack{\{u,v\}\subseteq V\\ D_{uv}=1}} D_{uv} = 2\sum_{\substack{\{u,v\}\subseteq V\\ D_{uv}=1}} 1 = 2\binom{k}{2}m = k(n-1)$$

and

$$\begin{aligned}
2\sum_{\substack{\{u,v\}\subseteq V\\ D_{uv}\geq 2}} D_{uv} &= \sum_{u\in V}\sum_{\substack{v\in V\\ D_{uv}\geq 2}} D_{uv} \\
&= \sum_{\substack{u,w\in V\\ w\sim u}}\ \sum_{\substack{v\in V\\ D_{uv}=1+D_{wv}}} (1+D_{wv}) \\
&= \sum_{w\in V}\sum_{\substack{v\in V\\ v\neq w}} (d_w-1)(k-1)(1+D_{wv}) \\
&= (k-1)\sum_{u\in V}\sum_{v\in V}(d_u-1)(1+D_{uv}) - (k-1)\sum_{u\in V}(d_u-1) \\
&= (k-1)\sum_{u\in V}\sum_{v\in V} d_u - (k-1)\sum_{u\in V}\sum_{v\in V} 1 + (k-1)\sum_{u\in V}\sum_{v\in V} d_u D_{uv} \\
&\quad -(k-1)\sum_{u\in V}\sum_{v\in V} D_{uv} - (k-1)\sum_{u\in V} d_u + (k-1)n \\
&= (k-1)kmn - (k-1)n^2 + (k-1)DD(G) - 2(k-1)W(G) \\
&\quad -(k-1)km + (k-1)n \\
&= (k-1)DD(G) - 2(k-1)W(G) + n^2 - n - k(n-1).
\end{aligned}$$

Thus

$$\begin{aligned} 2W(G) &= 2\sum_{\substack{\{u,v\}\subseteq V\\ D_{uv}=1}} D_{uv} + 2\sum_{\substack{\{u,v\}\subseteq V\\ D_{uv}\geq 2}} D_{uv} \\ &= (k-1)DD(G) - 2(k-1)W(G) + n^2 - n, \end{aligned}$$

from which we have the desired result. ■

Theorem 2. *Let G be a k-uniform hypertree with n vertices, where $2 \leq k \leq n$. Then*

$$2(k-1)^2 Gut(G) = 2k^2 W(G) - k(n-1)(2n-1).$$

Proof. Note that

$$\begin{aligned} 2\sum_{\substack{\{u,v\}\in V\\ D_{uv}=1,2}} D_{uv} &= \sum_{u\in V}\sum_{\substack{v\in V\\ D_{uv}=1}} 1 + 2\sum_{u\in V}\sum_{\substack{v\in V\\ D_{uv}=2}} 1 \\ &= \sum_{u\in V} d_u(k-1) + 4\sum_{w\in V}\sum_{\substack{\{u,v\}\subseteq V\\ D_{uw}=D_{vw}=1}} 1 \\ &= \sum_{u\in V} d_u(k-1) + 4\sum_{w\in V}\binom{d_w}{2}(k-1)^2 \\ &= \sum_{u\in V} d_u(k-1) + 2\sum_{w\in V} d_w(d_w-1)(k-1)^2 \\ &= (k-1)\sum_{u\in V} d_u + 2(k-1)^2\sum_{u\in V} d_u(d_u-1) \end{aligned}$$

and

$$\begin{aligned} 2\sum_{\substack{\{u,v\}\in V\\ D_{uv}\geq 3}} D_{uv} &= \sum_{u\in V}\sum_{\substack{v\in V\\ D_{uv}\geq 3}} D_{uv} \\ &= \sum_{\substack{u\in V\\ w\sim u}}\sum_{\substack{v\in V\\ z\sim v\\ D_{uz}=D_{wv}=D_{wz}+1}} (D_{wz}+2) \\ &= \sum_{w\in V}\sum_{z\neq w}(d_w-1)(d_z-1)(k-1)^2(D_{wz}+2) \\ &= (k-1)^2\sum_{u\in V}\sum_{v\neq u}(d_u-1)(d_v-1)(D_{uv}+2). \end{aligned}$$

Since $\sum_{u\in V} d_u = \frac{k(n-1)}{k-1}$, we have

$$2W(G) = 2\sum_{\substack{\{u,v\}\in V\\ D_{uv}=1,2}} D_{uv} + 2\sum_{\substack{\{u,v\}\in V\\ D_{uv}\geq 3}} D_{uv}$$

$$
\begin{aligned}
&= (k-1)\sum_{u\in V} d_u + 2(k-1)^2\sum_{u\in V} d_u(d_u-1) - (k-1)^2\sum_{u\in V} 2(d_u-1)^2 \\
&\quad +(k-1)^2\sum_{u\in V}\sum_{v\in V}(d_u-1)(d_v-1)(D_{uv}+2) \\
&= (k-1)\sum_{u\in V} d_u + 2(k-1)^2\sum_{u\in V}(d_u-1) \\
&\quad +(k-1)^2\sum_{u\in V}\sum_{v\in V} d_u d_v D_{uv} - (k-1)^2\sum_{u\in V}\sum_{v\in V}(d_u+d_v)D_{uv} \\
&\quad +(k-1)^2\sum_{u\in V}\sum_{v\in V} D_{uv} + (k-1)^2\sum_{u\in V}\sum_{v\in V} 2d_u d_v - (k-1)^2\sum_{u\in V}\sum_{v\in V} 2(d_u+d_v) \\
&\quad +(k-1)^2\sum_{u\in V}\sum_{v\in V} 2 = (k-1)\sum_{u\in V} d_u + 2(k-1)^2\sum_{u\in V} d_u - 2(k-1)^2\sum_{u\in V} 1 \\
&\quad +2(k-1)^2 Gut(G) - 2(k-1)^2 DD(G) + 2(k-1)^2 W(G) \\
&\quad +2(k-1)^2\sum_{u\in V} d_u\sum_{v\in V} d_v - 4(k-1)^2\sum_{u\in V} d_u\sum_{v\in V} 1 + 2(k-1)^2\sum_{u\in V}\sum_{v\in V} 1 \\
&= 2(k-1)^2 Gut(G) - 2(k-1)^2 DD(G) + 2(k-1)^2 W(G) \\
&\quad +k(n-1) + 2(k-1)k(n-1) - 2(k-1)^2 n \\
&\quad +2k^2(n-1)^2 - 4(k-1)kn(n-1) + 2(k-1)^2 n^2 \\
&= 2(k-1)^2 Gut(G) - 2(k-1)^2 DD(G) + 2(k-1)^2 W(G) \\
&\quad +2n^2 - (k+2)n + k,
\end{aligned}
$$

implying that

$$
\begin{aligned}
2(k-1)^2 Gut(G) &= 2(k-1)^2 DD(G) - 2(k-1)^2 W(G) + 2W(G) \\
&\quad -2n^2 + (k+2)n - k.
\end{aligned}
$$

From this formula and Theorem 1, we have

$$
\begin{aligned}
2(k-1)^2 Gut(G) &= 2(k-1)(2kW(G) - n(n-1)) \\
&\quad -2(k-1)^2 W(G) + 2W(G) - 2n^2 + (k+2)n - k \\
&= 2k^2 W(G) - k(n-1)(2n-1),
\end{aligned}
$$

as desired. ■

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