Properties of Degree Distance and Gutman Index of Uniform Hypergraphs

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Abstract

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, \( W(G) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} D_{uv} \). 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, \( DD(G) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} (d_u + d_v)D_{uv} = \sum_{u \in V} d_u \sum_{v \in V} D_{uv} \). 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, \( Gut(G) = \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_u d_v D_{uv} \). 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 \(\sum_{u \in V} d_u = km\). Note that
\[2 \sum_{\{u,v\} \subseteq V \atop D_{uv} = 1} D_{uv} = 2 \sum_{\{u,v\} \subseteq V \atop D_{uv} = 1} 1 = 2 \binom{k}{2} m = k(n - 1),\]
and
\[2 \sum_{\{u,v\} \subseteq V \atop D_{uv} \geq 2} D_{uv} = \sum_{u \in V} \sum_{v \in V} D_{uv} \geq 2 \sum_{u \in V} \sum_{v \in V} D_{uv} = \sum_{u,w \in V \atop w \sim u} \sum_{v \in V} D_{uv} = 1 + \sum_{u \in V} \sum_{v \in V} D_{uv} = \sum_{u \in V} \sum_{v \in V} (d_u - 1)(k - 1)(1 + D_{uv}).\]

\[= (k - 1) \sum_{u \in V} \sum_{v \in V} (d_u - 1)(1 + D_{uv}) - (k - 1) \sum_{u \in V} (d_u - 1)\]
\[= (k - 1) \sum_{u \in V} \sum_{v \in V} d_u - (k - 1) \sum_{u \in V} \sum_{v \in V} 1 + (k - 1) \sum_{u \in V} \sum_{v \in V} d_u D_{uv} - (k - 1) \sum_{u \in V} \sum_{v \in V} D_{uv} - (k - 1) \sum_{u \in V} d_u + (k - 1)n\]
\[= (k - 1)kmn - (k - 1)n^2 + (k - 1)DD(G) - 2(k - 1)W(G) - (k - 1)km + (k - 1)n\]
\[= (k - 1)DD(G) - 2(k - 1)W(G) + n^2 - n - k(n - 1).\]
Thus

\[ 2W(G) = 2 \sum_{\{u,v\} \subseteq V \atop D_{uw} = 1} D_{uv} + 2 \sum_{\{u,v\} \subseteq V \atop D_{uw} \geq 2} D_{uv} \]

\[ = (k - 1)DD(G) - 2(k - 1)W(G) + n^2 - n, \]

from which we have the desired result.

\[ \text{Theorem 2. Let } G \text{ be a } k\text{-uniform hypertree with } n \text{ vertices, where } 2 \leq k \leq n. \text{ Then} \]

\[ 2(k - 1)^2 \text{Gut}(G) = 2k^3W(G) - k(n - 1)(2n - 1). \]

\[ \text{Proof. Note that} \]

\[ 2 \sum_{\{u,v\} \subseteq V \atop D_{uw} = 1, 2} D_{uv} = \sum_{u \in V} \sum_{v \in V \atop D_{uw} = 1} 2 \sum_{u \in V} \sum_{v \in V \atop D_{uw} = 2} 1 \]

\[ = \sum_{u \in V} d_u(k - 1) + 4 \sum_{u \in V} \sum_{v \in V \atop \{u,v\} \subseteq V \atop D_{uw} = D_{vw} = 1} 1 \]

\[ = \sum_{u \in V} d_u(k - 1) + 4 \sum_{u \in V} \left( \frac{d_u}{2} \right) (k - 1)^2 \]

\[ = \sum_{u \in V} d_u(k - 1) + 2 \sum_{u \in V} d_u(d_u - 1)(k - 1)^2 \]

\[ = (k - 1) \sum_{u \in V} d_u + 2(k - 1)^2 \sum_{u \in V} d_u(d_u - 1) \]

and

\[ 2 \sum_{\{u,v\} \subseteq V \atop D_{uv} \geq 3} D_{uv} = \sum_{u \in V} \sum_{v \in V \atop D_{uv} \geq 3} D_{uv} \]

\[ = \sum_{u \in V} \sum_{v \in V \atop u \sim v \atop D_{uw} = D_{uv} - 1} (D_{uwz} + 2) \]

\[ = \sum_{u \in V} \sum_{z \in V \atop z \not= u \atop D_{uw} = D_{uv} = D_{uz} + 1} (d_w - 1)(d_z - 1)(k - 1)^2(D_{uwz} + 2) \]

\[ = (k - 1)^2 \sum_{u \in V} \sum_{v \in V \atop v \not= u} (d_u - 1)(d_v - 1)(D_{uv} + 2). \]

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

\[ 2W(G) = 2 \sum_{\{u,v\} \subseteq V \atop D_{uw} = 1, 2} D_{uv} + 2 \sum_{\{u,v\} \subseteq V \atop D_{uw} \geq 3} D_{uv} \]
\begin{align*}
&= (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} 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 \text{Gut}(G) - 2(k - 1)^2 DD(G) + 2(k - 1)^2 W(G) \\
&\quad + 2(k - 1)^2 \sum_{u \in V} \sum_{v \in V} d_u d_v - 4(k - 1)^2 \sum_{u \in V} \sum_{v \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 \text{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 \text{Gut}(G) - 2(k - 1)^2 DD(G) + 2(k - 1)^2 W(G) \\
&\quad + 2n^2 - (k + 2)n + k,
\end{align*}

implying that

\[ 2(k - 1)^2 \text{Gut}(G) = 2(k - 1)^2 DD(G) - 2(k - 1)^2 W(G) + 2W(G) \]
\[ -2n^2 + (k + 2)n - k. \]

From this formula and Theorem 1, we have

\[ 2(k - 1)^2 \text{Gut}(G) = 2(k - 1)(2kW(G) - n(n - 1)) \]
\[ -2(k - 1)^2 W(G) + 2W(G) - 2n^2 + (k + 2)n - k \]
\[ = 2k^2 W(G) - k(n - 1)(2n - 1), \]

as desired.
References


