Molecular Structure Descriptors for Volkmann Trees

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Abstract

For many molecular structure descriptors the Volkmann tree \( V_{n,d} \) is extremal among \( n \)-vertex trees in which no vertex has degree greater than \( d \). For this important class of (molecular) graphs, formulas for the general sum-connectivity, geometric-arithmetic index and Wiener polarity indices are given.

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1 The Volkmann Trees

Let \( G \) be a connected graph with the vertex-set \( V(G) \) and edge-set \( E(G) \), respectively. \( |V(G)| = n \), \( |E(G)| = m \) are the number of vertices and edges. The degree of a vertex \( v \in V(G) \) is the number of vertices joining to \( v \) and denoted by \( \text{deg}(v) \) (or simply as \( d_G(v) \), \( d(v) \)) and \( d_G(u, v) \) denote the degree of \( u \) and the distance (i.e., the number of edges on the shortest path) between \( u \) and \( v \), respectively.

In this paper we outline properties of a special type of trees which, for reasons explained later, are referred to as the Volkmann trees. The Volkmann tree \( V_{n,d} \) of order \( n \) and degree \( d \) is constructed as follows[1,2]:

Define \( n_i \) as 
\[ n_i = 1 + \sum_{j=1}^{i} d(d-1)^{j-1} \] for \( i = 1, 2, \cdots \). Choosing \( k \) such that \( n_{k-1} < n \leq n_k \), and calculating the parameters \( m \) and \( h \) from \( m = \left\lfloor \frac{n-n_{k-1}}{d-1} \right\rfloor \) and \( h = n - n_{k-1} - m(d-1) \). The vertices of \( V_{n,d} \) are arranged into \( k+1 \) levels. In level 0 there is one vertex, labeled by \( v_{0,1} \). In level \( i(i = 1, 2, \cdots, k-1) \), there are \( d(d-1)^i \) vertices, labeled by \( v_{i,1}, v_{i,2}, \cdots, v_{i,d(d-1)^{i-1}} \). These are connected
(in that order) to the vertices in level \( i - 1 \), so that \( d - 1 \) vertices from level \( i \) are adjacent to each vertex from level \( i - 1 \). At level \( k \) there are \( n - n_{k-1} \) vertices, labeled by \( v_{k,1}, v_{k,2}, \ldots, v_{k,n-n_{k-1}} \). These are connected (in that order) to the vertices in level \( k - 1 \), so that \( d - 1 \) vertices from level \( k \) are adjacent to vertices \( v_{k-1,1}, v_{k-1,2}, \ldots, v_{k-1,m} \). The remaining \( h \) vertices at level \( k \) (if any) are connected to the vertex \( v_{k-1,m+1} \) in level \( k - 1 \). If \( n = 1, 2, \ldots, d + 1 \) then \( V_{n,d} \) is the \( n \)-vertex star.

## 2 Molecular Structure Descriptors

In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modeled by a graph, where the points represent the atoms, and the edges symbolize the covalent bonds. Relevant properties of these graph models are then studied, giving rise to numerical graph invariants. The parameters derived from this graph-theoretic model of a chemical structure are being used not only in QSAR studies pertaining to molecular design and pharmaceutical drug design, but also in the environmental hazard assessment of chemicals. Many such graph invariant topological indices have been studied. The first, and most well-known parameter, the Wiener index\[3\], was introduced in the late 1940s in an attempt to analyze the chemical properties of paraffins (alkanes). Numerous other indices have been defined, and more recently, indices such as general sum-connectivity\[4\], geometric-arithmetic index\[5\] and Wiener polarity indices\[6\] have also been considered.

The well-known Randić index (connectivity index), introduced by chemist Randić\[7\] in 1975, is a graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies. It is defined as the sum over all edges of the (molecular) graph of the terms \( (d_u d_v)^{-\frac{1}{2}} \), i.e.,

\[
R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-\frac{1}{2}} \quad (1)
\]

The sum-connectivity index of the graph \( G \), denoted by \( \chi(G) \), is defined as\[4, 8\]:

\[
\chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-\frac{1}{2}} \quad (2)
\]

The general sum-connectivity index is defined as\[4\]:

\[
\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha \quad (3)
\]

the general sum-connectivity index generalized both the sum-connectivity index and the first Zagrebian index.
In recent papers [6, 9], the so-called geometric-arithmetic index $GA$ was conceived and investigated, defined as

$$GA(G) = \sum_{e \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$  

(5)

The Wiener polarity index of a graph $G = (V, E)$, denoted by $W_P(G)$, is defined by [7, 10]:

$$W_P(G) = |\{(u, v) | d(u, v) = 3, u, v \in V\}|$$

(6)


The Randić and general Randić indices, Zagreb indices, and nullity as well as an asymptotic expression for energy of Volkman Tree $V_{n,d}$ were characterized in [2]. Here, in our note, we investigate the general sum-connectivity, geometric-arithmetic index and Wiener polarity indices for $V_{n,d}$.

## 3 The General Sum-connectivity Of Volkman Trees

A $i-$ vertex denotes a vertex degree $i$, and a $(j, k)-$edge stands for an edge connecting a $j-$vertex with a $k-$vertex, and let $n_i$ denote the number of $i-$vertex, $m_{jk}$ be the number of $(j, k)-$edge, respectively.

Then, the general sum-connectivity index of any graph $G$ with $n$ vertices is denoted by $n_i$ and $m_{jk}$, i.e.,

$$\chi_\alpha(G) = \sum_{1 \leq j \leq k \leq n-1} m_{jk}(j+k)^\alpha.$$  

Theorem 3.1 Let $V_{n,d}$ be the Volkmann Tree depicted in Figure 1, then

(1) If $n \leq d + 1$, then $\chi_\alpha(V_{n,d}) = (n-1)n^\alpha$;

(2) If $n > d + 1$, then

$$\chi_\alpha(V_{n,d}) = h(h + 2)^\alpha + (h + d + 1)^\alpha + [md + d(d-1)^{k-2} - 2m - 1](d + 1)^\alpha + [n - md - d(d-1)^{k-2} + 2m - h - 1](2d)^\alpha.$$  

Proof. (1) If $n \leq d + 1$, then $V_{n,d}$ is the $n$-vertex star. By definition,

$$\chi_\alpha(V_{n,d}) = \sum_{1 \leq j \leq k \leq n-1} m_{jk}(j+k)^\alpha = (n-1)n^\alpha$$

(2) If $n > d + 1$, then there are four types of edges $e = uv$ in $V_{n,d}$, i.e., type 1: $(1, d)-$ edge; type 2: $(d, h+1)-$ edge; type 3: $(1, h+1)-$edge; and type 4: $(d, d)-$edge. In order to calculate the general sum-connectivity of $V_{n,d}$, we need to know the number of edges of each type.
(2.1) There are $m(d-1)$ edges connecting vertex of degree 1 with vertex of degree $d$ between level $k$ and level $k-1$, and there are also $n_{k-1} - n_{k-2} - m - 1$ such edges between level $k-1$ and level $k-2$, thus the number of edges of type 1 is $md + d(d-1)^{k-2} - 2m - 1$.

(2.2) Similarly, there is only 1 edge connecting vertex of degree $h+1$ with vertex of degree $d$.

(2.3) There are $h$ edges connecting vertex of degree 1 with vertex of degree $h+1$.

(2.4) There are $n - md - d(d-1)^{k-2} + 2m - h - 1$ edges connecting vertex of degree $d$ with vertex of degree $d$.

Thus, by definition of the general sum-connectivity index, $\chi_\alpha(V_{n,d})$ can be immediately obtained, as shown in Theorem 3.1.

4 The Geometric-arithmetic Of Volkman Trees

Based on the proof of Theorem 3.1, we arrive at

**Theorem 4.1** Let $V_{n,d}$ be a Volkmann tree of order $n$ and degree $d$,
(1) If $n \leq d + 1$, then $GA(V_{n,d}) = \frac{2(n-1)\sqrt{n-1}}{n}$;
(2) If $n > d + 1$, then

$$GA(V_{n,d}) = \frac{2h\sqrt{h+1}}{h+2} + \frac{2\sqrt{d(h+1)}}{h+d+1} + [md + d(d-1)^{k-2} - 2m - 1] \frac{2\sqrt{d}}{d+1}$$

$$+ n - md - d(d-1)^{k-2} + 2m - h - 1$$

**Proof.** We omit the proof here.

5 The Wiener Polarity Index Of Volkman Trees

Following by the definition of the Wiener polarity index, the Wiener polarity index of trees can be simplified as

**Lemma 5.1** ([6,10]). Let $T = (V, E)$ be a tree, Then

$$W_p(T) = \sum_{uv \in E} (d_T(u) - 1)(d_T(v) - 1) = \sum_{1 \leq i \leq j \leq n-1} (i-1)(j-1)m_{ij}$$

(7)

Similar to the proof of Theorem 3.1 and Theorem 4.1, we obtain

**Theorem 5.2** Let $V_{n,d}$ be a Volkmann tree of order $n$ and degree $d$,
(1) If $n \leq d + 1$, then $W_p(V_{n,d}) = 0$;
(2) If $n > d + 1$, then

$$W_p(V_{n,d}) = h(d-1) + [n - md - d(d-1)^{k-2} + 2m - h - 1](d-1)^2$$
Proof. (1) \( n \leq d + 1 \).

\( V_{n,d} \) is the \( n \)-vertex star. From formula (7), for the pendent edges, \( W_p = 0 \). 

(2) \( n > d + 1 \).

For the \((1, h+1)\), \((1, d)\)-edges, \( W_p = 0 \). Therefore, we only need to calculate the Wiener polarity index of edge such as \((d, h+1)\)-edge and \((d, d)\)-edge. \( m_{d,h+1} = 1, \ m_{d,d} = n - md - d(d - 1)^{k-2} + 2m - h - 1 \). Substituting into (8), we get the desired result.

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References


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