Volkmann Trees and Their Molecular Structure Descriptors*

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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. The definition of Volkman trees is provided and exemplified. For this important class of (molecular) graphs, formulas for the Randić and general Randić indices, Zagreb indices, and nullity are given, as well as an asymptotic expression for energy.

1 The Volkmann trees

Let G be a finite and undirected simple graph, with vertex set $V(G)$ and edge set $E(G)$. By n is denoted the order (= number of vertices, $|V(G)|$) of G. If G is connected and $|E(G)| = |V(G)| - 1$, then G is said to be a tree. 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:

If $n = 1, 2, \ldots, d+1$ then $V_{n,d}$ is the n-vertex star.

Let $n > d+1$. Define n_i as

$$n_i = 1 + \sum_{j=1}^{i} d(d-1)^{j-1} \qquad \text{for } i = 1, 2, \ldots.$$

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and choose k such that

$$n_{k-1} < n \leq n_k \ .$$

Then, calculate the parameters m and h from

$$m = \left\lfloor \frac{n - n_{k-1}}{d-1} \right\rfloor$$

and

$$h = n - n_{k-1} - (d-1)m \ .$$

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, $i = 1, 2, \ldots, k-1$, there are $d(d-1)^{i-1}$ vertices, labeled by $v_{i,1}, v_{i,2}, \ldots, v_{i,d(d-1)^{i-1}}$. 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 $k-1$.

Although the above specified construction of the Volkmann trees looks prohibitively complicated, these trees have a quite "reasonable" structure. This is illustrated in Figs. 1 and 2.

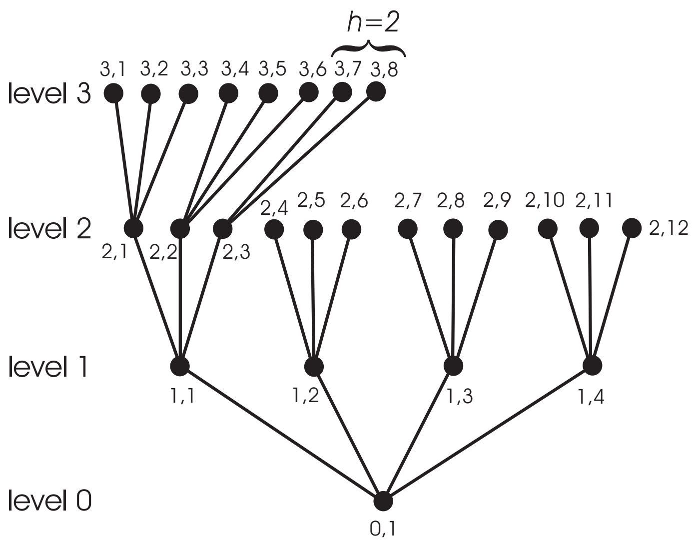

Fig. 1. The Volkmann tree $V_{25,4}$ and the labeling of its vertices.

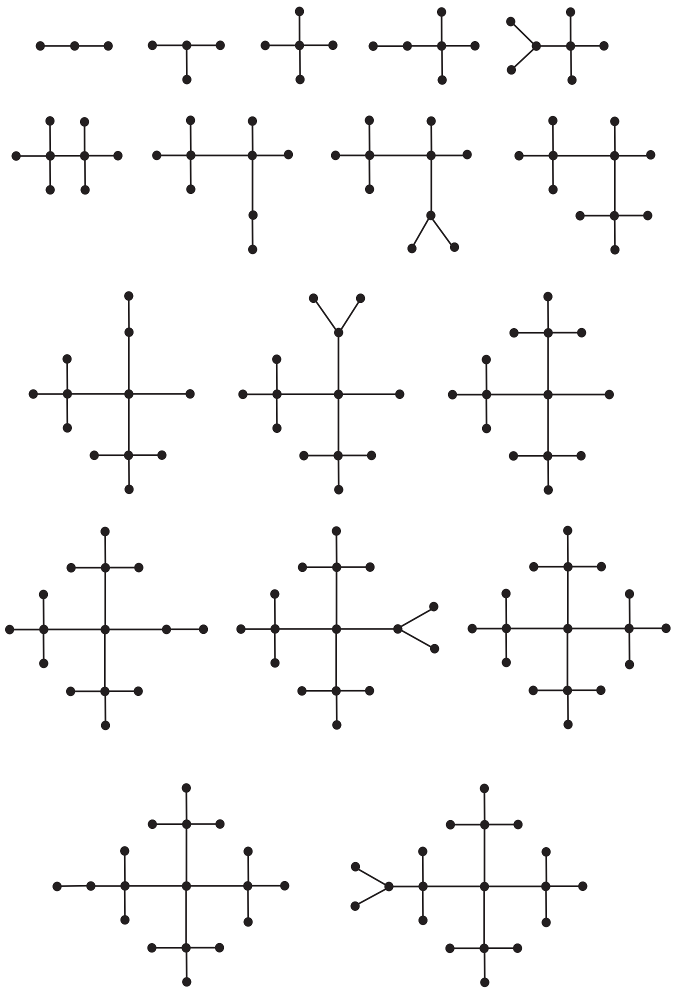

Fig. 2. The Volkmann trees $V_{n,4}$ for $n = 3, 4, \ldots, 19$.

2 Volkmann trees as extremal trees

Denote by $\mathcal{T}(n, d)$ the set of trees with n vertices in which no vertex has degree greater than d. From a chemical point of view, the set $\mathcal{T}(n, 4)$ is of outstanding importance, because this is just the set of the molecular graphs of all alkanes with n carbon atoms; the elements of $\mathcal{T}(n, 4)$ are usually referred to as *chemical trees*.

A problem often encountered in chemical graph theory is to characterize the chemical trees that are extremal with regard to some topological index TI. In a more formal way, one looks for trees $T_n^{min} \in \mathcal{T}(n, 4)$ and $T_n^{max} \in \mathcal{T}(n, 4)$, such that

$$TI(T_n^{min}) \leq TI(T_n) \leq TI(T_n^{max}) \tag{2.1}$$

holds for all $T_n \in \mathcal{T}(n,4)$. In "pure" graph theory the restriction $d = 4$ sounds unnecessary, and there one looks for trees $T_n^{min} \in \mathcal{T}(n,d)$ and $T_n^{max} \in \mathcal{T}(n,d)$, such that the relations (2.1) hold for all $T_n \in \mathcal{T}(n,d)$ and for some particular value (or, if possible, for all values) of the parameter d.

The n-vertex path P_n is element of any set $\mathcal{T}(n,d)$. For countless topological indices [1], P_n is one of the extremal graphs occurring in (2.1). For instance, P_n has maximal Wiener index [2], Hosoya index [3], Schultz index [4], hyper-Wiener index [5], energy [3], and Estrada index [6], as well as minimal Randić index [7], spectral radius [8], Laplacian spectral radius [9], to mention just a few.

Finding the other extremal tree in (2.1) appears to be a much more difficult task. In the case of the Wiener index, a computer-aided search for such trees was conducted in the 1990s [10]. However, it was the research group of Lutz Volkmann from Aachen, Germany [11] which gave a complete characterization of this tree. The chemical relevance of this result was then pointed out in [12]. Very soon after the publication of Volkmann's work [11], the same result was obtained also by Jelen and Triesch [13] (with giving due credit to Volkmann et al. for priority).[†]

Using the notation introduced in the previous section, we thus have the following:

Theorem 2.1. *Let $W(G)$ be the Wiener index (= sum of distances between all pairs of vertices) of the graph G. Then for any $n \geq 4$ and $d \geq 3$,*

$$W(V_{n,d}) \leq W(T_n) \leq W(P_n)$$

holds for any tree $T_n \in \mathcal{T}(n,d)$. Moreover,

$$W(V_{n,d}) < W(T_n) < W(P_n)$$

holds for any tree $T_n \in \mathcal{T}(n,d) \setminus \{P_n, V_{n,d}\}$.

After the discovery of Theorem 2.1, the fact that $TI(V_{n,d})$ is extremal in the class of trees $\mathcal{T}(n,d)$ was confirmed for several other topological indices TI. Simić and Tošić [14] proved this for the spectral radius, confirming thus the earlier empirical findings communicated in [12]. Recently Yu and Lu [15] did the same for the Laplacian spectral radius, confirming the earlier empirical findings communicated in [16,17]. It was claimed

[†]It is remarkable that Professors Volkmann and Triesch work at the same Mathematics Department and have offices quite close to each other.

(but not rigorously proven) that Volkmann trees are extremal also with regard to the Estrada index [18]. Volkmann trees are found to be extremal also in the case of Randić index [12] and eccentric connectivity index [19], but for these structure descriptors $V_{n,d}$ in not the unique extremal species.

The fact that Volkmann trees are not extremal for all topological indices – in particular for energy and Hosoya index – was noticed already in [12] and finally settled by Heuberger and Wagner [20–22].

From the material presented in this section it should be evident why Volkmann trees deserve attention of scholars doing research in chemical graph theory. In what follows we establish a few of their properties.

3 Randić and general Randić indices of Volkmann trees

The Randić index $R(G)$ of a graph G is defined as the sum of the terms $1/\sqrt{d_u d_v}$ over all edges uv of G, where d_u denotes the degree of $u \in V(G)$, i. e.,

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u\, d_v}} \, .$$

Historically, $R(G)$ was introduced by Randić [23] in 1975 as one of the first molecular–graph–based structure descriptors (cf. [1]). Since then it found countless applications (see, e. g., [24–26]) and its theory became one of the most prolific areas of chemical graph theory (see, e. g., [27, 28]). In this section we give the formula for calculating the Randić index of the Volkmann trees.

Theorem 3.1. *Let $V_{n,d}$ be a Volkmann tree of order n and degree d.*
(1) If $n \leq d+1$, then $R(V_{n,d}) = \sqrt{n-1}$.
(2) If $n > d+1$, then

$$\begin{aligned} R(V_{n,d}) &= \frac{h}{\sqrt{h+1}} + \frac{1}{\sqrt{d(h+1)}} + \frac{md + n_{k-1} - 2m - 1}{\sqrt{d}} \\ &+ \frac{n - md - n_{k-1} + 2m - h - 1}{d} \, . \end{aligned}$$

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

$$R(V_{n,d}) = \sum_{uv \in V_{n,d}} \frac{1}{\sqrt{d_u d_v}} = \frac{n-1}{\sqrt{n-1}} = \sqrt{n-1} \, .$$

(2) If $n > d+1$, then there are four types of edges $e = uv$ in $V_{n,d}$, i. e., type 1: $d_u = 1$, $d_v = d$; type 2: $d_u = d$, $d_v = h+1$; type 3: $d_u = 1$, $d_v = h+1$; and type 4: $d_u = d, d_v = d$. In order to calculate the Randić index of $V_{n,d}$, we need to know the number of edges of each type.

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 $n_{k-1} - m - 1$ such edges between level $k-1$ and level $k-2$, thus the number of edges of type 1 is $md + n_{k-1} - 2m - 1$.

Similarly, there is only 1 edge connecting vertex of degree $h+1$ with vertex of degree d. There are h edges connecting vertex of degree 1 with vertex of degree $h+1$. And there are $n - md - n_{k-1} + 2m - h - 1$ edges connecting vertex of degree d with vertex of degree d. Thus, by definition of the Randić index, $R(V_{n,d})$ can be immediately obtained, as given in the theorem. □

The general Randić index is defined as [27]

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u\, d_v)^\alpha$$

where α is some real number. Evidently, the ordinary Randić index is the special case of the general Randić index for $\alpha = -1/2$. Repeating the reasoning from the proof of Theorem 3.1 we obtain:

Theorem 3.2. *Let $V_{n,d}$ be a Volkmann tree of order n and degree d.*
(1) If $n \leq d+1$, then $R_\alpha(V_{n,d}) = (n-1)^{\alpha+1}$.
(2) If $n > d+1$, then

$$\begin{aligned} R_\alpha(V_{n,d}) &= h(h+1)^\alpha + [d(h+1)]^\alpha + (md + n_{k-1} - 2m - 1)\, d^\alpha \\ &+ (n - md - n_{k-1} + 2m - h - 1)\, d^{2\alpha} . \end{aligned}$$

4 Zagreb indices of Volkmann trees

The first and second Zagreb indices of a graph G are defined as [1]

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d_u\, d_v .$$

The Volkmann tree $V_{n,h}$ has n_1 vertices of degree 1, n_d vertices of degree d and, if $h > 0$, one vertex of degree $h+1$. Suppose first that $h > 0$. Then

$$n_1 + n_d + 1 = n \qquad \text{and} \qquad n_1 + d\, n_d + (h+1) = 2(n-1)$$

from which follows

$$n_1 = n - 1 - \frac{n-h-2}{d-1} \qquad \text{and} \qquad n_d = \frac{n-h-2}{d-1} \ . \tag{4.2}$$

If $h = 0$ then instead of Eqs. (4.2) we get

$$n_1 = n - \frac{n-2}{d-1} \qquad \text{and} \qquad n_d = \frac{n-2}{d-1} \ .$$

By means of these formulas we obtain

Theorem 4.1. *Let $V_{n,d}$ be a Volkmann tree of order n and degree d.*
(1) If $n \leq d+1$, then $M_1(V_{n,d}) = n(n-1)$.
(2) If $n > d+1$ and $h = 0$, then

$$M_1(V_{n,d}) = n - \frac{n-2}{d-1} + \frac{n-2}{d-1}\, d^2 \ .$$

(3) If $n > d+1$ and $h > 0$, then

$$M_1(V_{n,d}) = n - 1 - \frac{n-h-2}{d-1} + \frac{n-h-2}{d-1}\, d^2 + (h+1)^2 \ .$$

Comparing the definitions of the general Randić index and the second Zagreb index, it is seen that $M_2(G) \equiv R_\alpha(G)$ for $\alpha = 1$. In view of this, from Theorem 3.2 directly follows:

Theorem 4.2. *Let $V_{n,d}$ be a Volkmann tree of order n and degree d.*
(1) If $n \leq d+1$, then $M_2(V_{n,d}) = (n-1)^2$.
(2) If $n > d+1$, then

$$\begin{aligned} M_2(V_{n,d}) &= h(h+1) + d(h+1) + (md + n_{k-1} - 2m - 1)\, d \\ &+ (n - md - n_{k-1} + 2m - h - 1)\, d^2 \ . \end{aligned}$$

5 Asymptotic behavior of the energy of Volkmann trees

From now on the vertices of the graph G will be labeled by $v_1, v_2, \ldots, v_n$. Then the adjacency matrix $\mathbf{A}(G)$ of G is the square matrix of order n, whose (i,j)-entry is equal to 1 if the vertices v_i and v_j are adjacent, and is equal to zero otherwise. The characteristic polynomial of the adjacency matrix, $\phi(G,x) = det(x\,\mathbf{I}_n - \mathbf{A}(G))$, is said to be the characteristic polynomial of the graph G. The eigenvalues of a graph G are defined as the eigenvalues of its adjacency matrix, and so these are just the roots of the equation $\phi(G,x) = 0$. Denote them by $\lambda_1, \lambda_2, \ldots, \lambda_n$, and as a whole they form the spectrum of G, denoted by $Spec(G)$. Then the energy of G is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \ .$$

For details on graph energy see [29, 30].

Let $m(G,k)$ be the number of matchings of size k of G. Then, if G is a tree,

$$\phi(G,x) = \sum_{k \geq 0} (-1)^k \, m(G,k) \, x^{n-2k}$$

and

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{k \geq 1} m(G,k) \, x^{2k} \right] dx \ .$$

The matching polynomial is defined as [31]

$$M(T,x) = \sum_k m(T,k) \, x^k \ .$$

In [22] Heuberger and Wagner determined the asymptotic behavior of the energy of a kind of special trees. These trees are similar, but not identical to Volkmann trees. Here we show that similar methods can be used to obtain the asymptotic behavior of the energy of Volkmann trees.

In order to state our result, we use the notion of complete d-ary trees: The complete d-ary tree of height $h-1$ is denoted by C_h^d, i. e., C_1^d is a single vertex and C_h^d has d branches $C_{h-1}^d, \ldots, C_{h-1}^d$ (see Fig. 3).

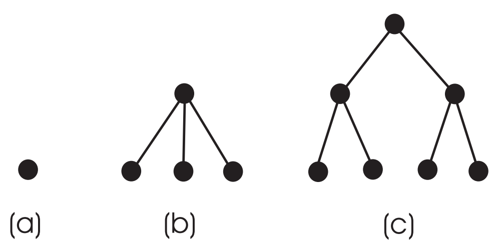

Fig. 3. Complete d-ary trees; (a) C_1^d for all d, (b) C_2^3, (c) C_3^2.

It is convenient to set C_0^d to be the empty graph. Then $V_{n,d}$ can be decomposed as shown in Fig. 4, where $B_{i,j} \in \{C_{k-i}^{d-1}, C_{k-i-1}^{d-1}\}$ for $0 \leq i \leq k-1$.

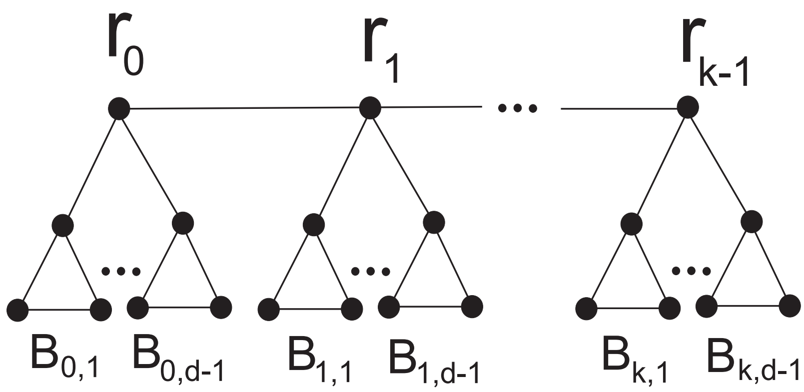

Fig. 4. Decomposition of the Volkmann tree.

Theorem 5.1. *The energy of $V_{n,d}$ is asymptotically equal to*

$$E(V_{n,d}) = \alpha_{d-1}\, n + O(\log n)$$

where

$$\alpha_{d-1} = 2\sqrt{d-1}(d-2)^2 \left[\sum_{\substack{j\geq 1 \\ j\equiv 0 (mod 2)}} (d-1)^{-j}(\cot\frac{\pi}{2j} - 1) + \sum_{\substack{j\geq 1 \\ j\equiv 1 (mod 2)}} (d-1)^{-j}(\csc\frac{\pi}{2j} - 1) \right]$$

is a constant that only depends on d.

In order to prove this theorem, we need the following lemma from [22]:

Lemma 5.2. *The energy of a complete d-ary tree C_h^d satisfies*

$$E(C_h^d) = \alpha_d |C_h^d| + O(1)$$

where $|C_h^d|$ denotes the number of vertices of C_h^d and

$$\alpha_d = 2\sqrt{d}(d-1)^2 \left[\sum_{\substack{j\geq 1 \\ j\equiv 0 (mod 2)}} d^{-j}(\cot\frac{\pi}{2j} - 1) + \sum_{\substack{j\geq 1 \\ j\equiv 1 (mod 2)}} d^{-j}(\csc\frac{\pi}{2j} - 1) \right]$$

is a constant that only depends on d.

Now, we are able to prove our main asymptotic result.

Proof of Theorem 5.1. Using the decomposition of $V_{n,d}$ as shown in Fig. 4, we note that

$$\left(\prod_{j=1}^{d-1} M(B_{0,j},x)\right)\left(\prod_{i=1}^{k-2}\prod_{j=1}^{d-2} M(B_{i,j},x)\right)\left(\prod_{j=1}^{d-1} M(B_{k-1,j},x)\right) \le M(V_{n,d},x)$$

$$\le \left(\prod_{j=1}^{d-1} M(B_{0,j},x)\right)\left(\prod_{i=1}^{k-2}\prod_{j=1}^{d-2} (B_{i,j},x)\right)\left(\prod_{j=1}^{d-1} M(B_{k-1,j},x)\right)(1+x)^{dk}$$

for arbitrary $x > 0$, since every matching in the union $\bigcup_i \bigcup_j B_{i,j}$ is also a matching in $V_{n,d}$, whereas every matching of $V_{n,d}$ consists of a matching in $\bigcup_i \bigcup_j B_{i,j}$ and a subset of the remaining $\le dk$ edges. Since

$$\phi(T,x) = \sum_{k\ge 0} (-1)^k m(T,k)\, x^{n-2k} = x^n\, M(T,-x^{-2}),$$

this implies that

$$\sum_{j=1}^{d-1} E(B_{0,j}) + \sum_{i=1}^{k-2}\sum_{j=1}^{d-2} E(B_{i,j}) + \sum_{j=1}^{d-1} E(B_{k-1,j}) \le E(V_{n,d})$$

$$\le \sum_{j=1}^{d-1} E(B_{0,j}) + \sum_{i=1}^{k-2}\sum_{j=1}^{d-2} E(B_{i,j}) + \sum_{j=1}^{d-1} E(B_{k-1,j}) + \frac{2}{\pi} dk \int_0^\infty x^{-2}\log(1+x^2)dx \ .$$

Since $\int_0^\infty x^{-2}\log(1+x^2)dx = \pi$, this implies that

$$\begin{aligned}
E(V_{n,d}) &= \sum_{j=1}^{d-1} E(B_{0,j}) + \sum_{i=1}^{k-2}\sum_{j=1}^{d-2} E(B_{i,j}) + \sum_{j=1}^{d-1} E(B_{k-1,j}) + O(k) \\
&= \sum_{j=1}^{d-1}(\alpha_{d-1}|B_{0,j}| + O(1)) + \sum_{i=1}^{k-2}\sum_{j=1}^{d-2}(\alpha_{d-1}|B_{i,j}| + O(1)) \\
&+ \sum_{j=1}^{d-1}(\alpha_{d-1}|B_{k-1,j}| + O(1)) + O(k) \\
&= \alpha_{d-1}\left(\sum_{j=1}^{d-1}|B_{0,j}| + \sum_{i=1}^{k-2}\sum_{j=1}^{d-2}|B_{i,j}| + \sum_{j=1}^{d-1}|B_{k-1,j}|\right) + O(k) \\
&= \alpha_{d-1}(|V_{n,d}| - k) + O(k) = \alpha_{d-1}\, n + O(k) \ .
\end{aligned}$$

It is not difficult to see that $k = O(\log n)$ by the definition of the Volkmann tree, and so we finally have $E(V_{n,d}) = \alpha_{d-1}\, n + O(\log n)$, which completes the proof. □

6 The nullity of the Volkmann tree

The nullity of a graph G, denoted by $n_0(G)$, is the multiplicity of the eigenvalue zero [32, 33]. We can get the nullity of a tree as follows [33]: Choose any leaf (= vertex of degree 1) of the tree, delete the leaf and its parent, repeat this operation until there remain only isolated vertices. Then the number of isolated vertices equals the nullity of the tree. The operation also finds a maximum matching, so we call the deleted vertices to be matched, and call the remaining vertices to be exposed.

We now use the decomposition of the Volkmann tree again, but with more details. Namely, we determine the explicit number of $B_{i,j}$ which equals to C_{k-i}^{d-1} for each vertex r_i.

Lemma 6.1. *Denote the number of $B_{i,j}$ which equal to C_{k-i}^{d-1} by a_i, then*

$$\begin{aligned}
a_0 &= \left\lceil \frac{n-n_{k-1}}{(d-1)^{k-1}} \right\rceil - 1 \\
a_1 &= \left\lceil \frac{n-n_{k-1}-a_0(d-1)^{k-1}}{(d-1)^{k-2}} \right\rceil - 1 \\
\cdots &\quad \cdots \\
a_i &= \left\lceil \frac{n-n_{k-1}-a_0(d-1)^{k-1}-a_1(d-1)^{k-2}-\cdots-a_{i-1}(d-1)^{k-i}}{(d-1)^{k-i-1}} \right\rceil - 1 \\
\cdots &\quad \cdots \\
a_{k-1} &= n-n_{k-1}-a_0(d-1)^{k-1}-a_1(d-1)^{k-2}-\cdots-a_{k-2}(d-1)\ .
\end{aligned}$$

Proof. The number of the vertices on level k of the Volkmann tree is $n-n_{k-1}$, and the number of the vertices of level k of a complete $d-1$-ary tree is $(d-1)^{k-1}$, and so, for vertex r_0, the number of branches equal to C_k^{d-1} is $\left\lfloor \frac{n-n_{k-1}}{(d-1)^{k-1}} \right\rfloor$, when $\frac{n-n_{k-1}}{(d-1)^{k-1}}$ is not an integer. Note that if $\frac{n-n_{k-1}}{(d-1)^{k-1}}$ is an integer, then r_0 has actually $\frac{n-n_{k-1}}{(d-1)^{k-1}}$ branches equal to C_k^{d-1}, but we will regard the root of any of C_k^{d-1} as r_1, so there are $\frac{n-n_{k-1}}{(d-1)^{k-1}}-1$ fragments $B_{0,j}$ which equals to C_k^{d-1}. From the above, $a_0 = \left\lceil \frac{n-n_{k-1}}{(d-1)^{k-1}} \right\rceil - 1$. Other $a_i's$ can be calculated similarly. $\square$

Next, we calculate the nullity of a complete $d-1$-ary tree of height $h-1$.

Lemma 6.2.

$$n_0(C_h^{d-1}) = \begin{cases} \dfrac{(d-1)^{h-1}-1}{d} & \textit{for } h \textit{ even} \\[2ex] \dfrac{(d-1)^{h-1}+1}{d} & \textit{for } h \textit{ odd} \end{cases}$$

Proof. When we delete a leaf vertex on level k, at the same time, we delete its parent on level $k-1$, there are $d-2$ isolated vertices left. Since there are $(d-1)^{k-2}$ vertices on level $k-1$, we can delete $(d-1)^{k-2}$ leaf vertices on level k, and hence there are $(d-2)(d-1)^{k-2}$ isolated vertices left together with a C_{k-2}^{d-1}. Similarly, when we delete the $(d-1)^{i-2}$ leaf vertices on level i and their parents on level $i-1$, there are $(d-2)(d-1)^{i-2}$ new isolated vertices left together with a C_{i-2}^{d-1}, where $2 \le i \le k$ and $i \equiv k (mod\ 2)$. Obviously, $n_0(C_0^{d-1}) = 0$ and $n_0(C_1^{d-1}) = 1$. By adding the number of the new isolated vertices left after every deletion, we are done. □

Therefore, for a Volkmann tree, we can calculate its nullity as follows.

For r_0, we consider the subtree consisting of r_0 and its branches, denoted by T_0. Denote the roots of the branches by $t_{0_1}, t_{0_2}, \ldots, t_{0_{d-1}}$, respectively. We delete the leaf vertices and their parents repeatedly.

Finally, if r_0 is deleted, namely, for some t_{0_j}, t_{0_j} was exposed in the branch containing it, but matched with r_0 in T_0. So the number of exposed vertices in T_0 is by one less than the sum of the number of exposed vertices in the branches of r_0, and hence $b_0 = -1$. To be this case, there must be a branch equal to C_k^{d-1}, if k is odd, C_{k-1}^{d-1}, if k is even, which is equivalent to $d-1 \ge a_0 \ge 1$, if k is odd, and $0 \le a_0 \le d-2$, if k is even. Once r_0 is deleted, we can delete T_0 from the decomposition, and then consider the remainder of the tree similarly. The only thing that needs to be noticed is that the number of branches of r_i is $d-2$ for $1 \le i \le k-2$, and so the range of a_i is a bit different.

If all t_{0_j} are matched in their own branches, then r_0 becomes an isolated vertex in T_0, also a leaf vertex in $V_{n,d}$. So we can match r_0 with r_1 (delete r_0 and r_1). In this case, the number of exposed vertices in $T_0 \bigcup T_1$ is exactly the sum of the number of exposed vertices in the branches of r_0 and r_1. Namely, $b_0 + b_1 = 0$. To be this case there must be no branch equal to C_k^{d-1}, if k is odd, C_{k-1}^{d-1}, if k is even, which is equivalent to $a_0 = 0$, if k is odd, and $a_0 = d-1$, if k is even. Once r_0 and r_1 are deleted, we can delete T_0 and T_1 from the decomposition, and then consider the remainder of the tree similarly. Again, pay attention to the range of a_i for $2 \le i \le k-2$.

From the above discussion, we can give recursive expressions for the case k is even as follows. (The case k is odd is similar.)

Lemma 6.3. $\sum_{i=0}^{k-1} b_i$ *can be calculated recursively as follows:*

$$b_0 + b_1 + \cdots + b_{k-1} = \begin{cases} -1 + b_1 + \cdots + b_{k-1} & 0 \le a_0 \le d-2 \\ b_2 + \cdots + b_{k-1} & a_0 = d-1 \end{cases}$$

$$b_1 + \cdots + b_{k-1} = \begin{cases} -1 + b_2 + \cdots + b_{k-1} & 1 \le a_1 \le d-2 \\ b_3 + \cdots + b_{k-1} & a_1 = 0 \end{cases}$$

$$b_2 + \cdots + b_{k-1} = \begin{cases} -1 + b_3 + \cdots + b_{k-1} & 0 \le a_2 \le d-3 \\ b_4 + \cdots + b_{k-1} & a_2 = d-2 \end{cases}$$

$$\cdots \qquad \cdots$$

$$b_{2i-1} + \cdots + b_{k-1} = \begin{cases} -1 + b_{2i} + \cdots + b_{k-1} & 1 \le a_{2i-1} \le d-2 \\ b_{2i+1} + \cdots + b_{k-1} & a_{2i-1} = 0 \end{cases}$$

$$b_{2i} + \cdots + b_{k-1} = \begin{cases} -1 + b_{2i+1} + \cdots + b_{k-1} & 0 \le a_{2i} \le d-3 \\ b_{2i+2} + \cdots + b_{k-1} & a_{2i} = d-2 \end{cases}$$

$$\cdots \qquad \cdots$$

$$b_{k-2} + b_{k-1} = \begin{cases} -1 + b_{k-1} & 0 \le a_{k-2} \le d-3 \\ 0 & a_{k-2} = d-2 \end{cases}$$

$$b_{k-1} = \begin{cases} -1 & a_{k-1} \ge 1 \\ 1 & a_{k-1} = 0 \end{cases}$$

We thus arrive at:

Theorem 6.4. *The nullity $n_0(V_{n,d})$ of the Volkmann tree $V_{n,d}$ is given by*

$$\begin{aligned} n_0(V_{n,d}) &= a_0\, n_0(C_k^{d-1}) + (d-1-a_0+a_1) n_0\,(C_{k-1}^{d-1}) \\ &+ (d-2-a_1+a_2) n_0\,(C_{k-2}^{d-1}) + \cdots + (d-2-a_{i-1}+a_i) n_0\,(C_{k-i}^{d-1}) \\ &+ \cdots + (d-2-a_{k-2}+a_{k-1}) n_0\,(C_1^{d-1}) + b_0 + b_1 + \cdots + b_{k-1} \end{aligned}$$

where a_i, $n_0(C_h^{d-1})$ and $\sum_{i=0}^{k-1} b_i$ are given in Lemmas 6.1, 6.2, and 6.3, respectively.

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