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Dendrimers are the Unique Chemical Trees with Maximum Spectral Radius

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Abstract

It is shown that dendrimers have maximum spectral radius and maximum Colatz-Sinogowitz index among all chemical trees of given size. The result is also generalized for the class of chemical trees with prescribed number of pendant vertices.

In chemical graph theory hydrocarbons are modeled by graphs in which no vertex has degree (or valency) larger than 4. In particular *chemical trees* represent alkanes [8]. There exists vast literature where topological indices are intensively studied and their relation to chemical properties are investigated. One of the most prominent among them is the spectral radius of the adjacency matrix $\lambda_1(G)$ of the underlying graph, often referred as *the index* of the graph [3]. Fischermann et al. [4] observed in their numerical experiments

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with trees that have maximum $\lambda_1(T)$ among all chemical trees with n vertices belong to the class of *dendrimers*. They conjecture that this is not a mere coincidence.

A *dendrimer* D_n is a chemical tree of order n that can be constructed by breadth-first search in the following way: Start with a root vertex v_0 at level 0 and connect it to at most s vertices v_1, \dots, v_s ($s \leq 4$) at level 1. By recursion each vertex at level k is connected to exactly $s - 1$ vertices in level $k + 1$ until all vertices are exhausted. (The last vertex in this procedure may have less than $s - 1$ neighbors in level $k + 1$.) This is done by iterating over all vertices in the order of their indices. Dendrimers are also extremal with respect to other topological indices, e.g., they are chemical trees with minimal Wiener index [5].

Gutman et al. [6] used the AutoGraphiX (AGX) System [1] and observed that dendrimers also maximize the closely related Collatz-Sinogowitz index for chemical trees with at most 29 vertices. The *Collatz-Sinogowitz* index for a tree T is given by

$$CS(T) = \lambda_1(T) - d_{av}(T) = \lambda_1(T) - 2 \frac{n - 1}{n}$$

where $d_{av}(T)$ denotes the average degree of T . Gutman et al. [6] conjectured that dendrimers D_n uniquely maximize $CS(T)$ for chemical trees for all n .

We give a formal proof for the above two conjectures.

Theorem 1. *Dendrimers are the unique chemical trees that have maximum spectral radius $\lambda_1(T)$ (and maximum Collatz-Sinogowitz index $CS(T)$) among all chemical trees with n vertices.*

We do so in applying a more general result on general trees. Let $G = (V, E)$ be a tree. Let $d(v)$ denote the degree of vertex v . A sequence $\pi = (d_1, \dots, d_n)$ of nonnegative integers in non-increasing order is called *degree sequence* if there exists a graph G with n vertices for which d_1, \dots, d_n are the degrees of its vertices. A sequence π is a *tree sequence* (i.e., the degree sequence of a tree) if and only if $d_i > 0$ for all $k = 1, \dots, n$ and $\sum_{k=1}^n d_i = 2(n - 1)$. Let \mathcal{T}_π be the set of all trees with degree sequence π .

Trees with maximum spectral radius in \mathcal{T}_π are unique up to isomorphism [2]. They can be constructed by a breadth-first search similar to dendrimers: Start with a root vertex v_0 at level 0 and connect it to d_1 vertices v_1, \dots, v_{d_1} at level 1. Then join the next $d_2 - 1$ vertices $v_{d_1+1}, \dots, v_{d_1+d_2-1}$ to v_1 , the next $d_3 - 1$ vertices $v_{d_1+d_2}, \dots, v_{d_1+d_2+d_3-2}$ to v_2 and so on to get all vertices in level 2. By recursion connect the vertices of level k to the vertices of level $k + 1$ until all vertices (and thus the degrees of the tree sequence)

are exhausted. Thus we get a well-ordering of the vertices. In [2] we have called such an ordering *breadth-first search ordering with decreasing degrees* (BFD-ordering for short) and trees that possess such an ordering a *BFD-tree*.

Proposition 2 ([2]). *A tree T with degree sequence π has maximum spectral radius in class \mathcal{T}_π if and only if it is a BFD-tree. T is then uniquely determined up to isomorphism.*

Observe that dendrimers are the unique BFD-trees for tree sequences $\pi = (4, \dots, 4, \alpha, 1, \dots, 1)$ where $\alpha \in \{1, 2, 3\}$.

The next result provides a partial ordering of tree classes with given degree sequences. A degree sequence $\pi = (d_1, \dots, d_n)$ is said to *majorize* a degree sequence $\pi' = (d'_1, \dots, d'_n)$ if $\sum_{i=1}^n d_i = \sum_{i=1}^n d'_i$ and $\sum_{i=1}^j d_i \geq \sum_{i=1}^j d'_i$ for all $j = 1, \dots, n$. We write $\pi' \triangleleft \pi$.

Proposition 3 ([2]). *Let π and π' be two distinct degree sequences of trees with $\pi' \triangleleft \pi$. Let T and T' be trees with maximum spectral radii in classes \mathcal{T}_π and $\mathcal{T}_{\pi'}$, resp. Then $\lambda(T') < \lambda(T)$.*

Proof of Theorem 1. Let $\pi = (d_1, \dots, d_n) = (4, \dots, 4, d_r, 1, \dots, 1)$ be the degree sequence of a dendrimer D_n . Then for any other tree sequence $\pi' = (d'_1, \dots, d'_n)$ we find $\pi' \triangleleft \pi$. Suppose this is not the case. Then there is an index s such that $\sum_{i=1}^s d_i < \sum_{i=1}^s d'_i$. By construction $d'_i \leq d_i = 4$ for all $i = 1, \dots, r - 1$ and $d'_i \geq d_i = 1$ for all $i = r + 1, \dots, n$. Thus $s \geq r$ and we have $2n - 2 = \sum_{i=1}^n d'_i = \sum_{i=1}^s d'_i + \sum_{i=s+1}^n d'_i > \sum_{i=1}^s d_i + \sum_{i=s+1}^n d_i = 2n - 2$, a contradiction. Since dendrimers have maximum index in their degree class by Proposition 2 the statement follows from Proposition 3. □

Remark 4. *The statement of Theorem 1 can also be deduced from a result by Simić and Tošić [7]. They showed that there is an unique d -regular tree that maximizes the largest eigenvalue for all trees of given size n and given maximum degree d and give a characterization of this unique tree. This result can be derived from Propositions 2 and 3 analogously to the proof of Theorem 1.*

Notice that the above arguments also allows to characterize trees with prescribed numbers of vertices of valency 1, 2, 3, and 4, resp., that have maximum index. For example, look at the class of chemical trees which have a given size n and a given number k of pendant vertices. Let n_j denote the number of vertices of degree j for $j = 1, \dots, 4$. By our assumption $n_1 = k$. It is then straightforward to compute that $\sum_{j=1}^4 j n_j = \sum_{i=1}^n d_i =$

$2n - 2 = 2 \sum_{j=1}^4 n_j - 2$ and hence $n_4 = (k - n_3)/2 - 1$. Thus analogously to the proof of Theorem 1 a chemical tree sequence π majorizes all other chemical tree sequences with $n_1 = k$ if and only if $n_3 = k \pmod 2$. Therefore we can derive the following result from Propositions 2 and 3.

Theorem 5. *A chemical tree has maximum spectral radius $\lambda_1(T)$ (and maximum Collatz-Sinogowitz index $CS(T)$) among all chemical trees with n vertices and k pendant vertices if and only if it is the (unique) BDF-tree with $n_3 = k \pmod 2$, $n_4 = (k - n_3)/2 - 1$, $n_2 = n - n_4 - n_3 - k$, and $n_1 = k$.*

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