Extremal k-ape Trees for Randić Index
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Abstract

The Randić (connectivity) index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies. A graph $G$ is called an apex tree if it contains a vertex $x$ such that $G - x$ is a tree. For any integer $k \geq 1$ the graph $G$ is called $k$-apex tree if there exists a subset $X$ of $V(G)$ of cardinality $k$ such that $G - X$ is a tree and for any $Y \subset V(G)$ and $|Y| < k$, $G - Y$ is not a tree. J. Gao [3] found the sharp upper bound for the Randić index of apex trees. In this paper, we proved that $k$-apex trees are not regular for $k \geq 2$ and proposed a sharp upper bound for the Randić index of $k$-apex trees for $k \geq 2$.

1 Introduction

In studying branching properties of alkanes, several numbering schemes for the edges of the associated hydrogen-suppressed graph were proposed based on the degrees of the end vertices of an edge [12]. To preserve rankings of certain molecules, some inequalities involving the weights of edges needed to be satisfied. Randić [12] stated that weighting all edges $uv$ of the associated graph $G$ by $(d(u)d(v))^{\frac{1}{2}}$ preserved these inequalities, where $d(u)$ and $d(v)$ are the degrees of vertices $u$ and $v$ respectively. The sum of weights over all edges of $G$, which is called the Randić index or molecular connectivity index or simply connectivity index of $G$ and denoted by $R(G)$, has been closely correlated with many chemical properties [7] and found to parallel the boiling point, Kovats constants, and a calculated surface. In addition, the Randić index appears to predict the boiling points of alkanes more closely, and only it takes into account the bonding or adjacency degree among carbons in alkanes [8]. It is said in [9] that Randić index together with its generalizations it is certainly the molecular-graph-based structure descriptor, that found the most numerous applications in organic chemistry, medicinal chemistry, and pharmacology. More data and additional references on the index can be found in [5, 4].

All graphs considered in this paper are simple, finite and connected. For a vertex $v \in V(G)$ its degree is denoted by $d_G(v)$ and if $G$ is clear from
the context we simplify the notation to \(d(v)\). For \(X \subset V(G)\), \(G - X\) is the subgraph of \(G\) obtained from \(G\) by removing the vertices of \(X\) and edges incident with them, in particular \(G - \{v\}\) is denoted by \(G - v\). An edge \(uv\) in \(G\) is called symmetric edge if \(d(u) = d(v)\). An edge which is not symmetric is called asymmetric.

The Randić index of the graph \(G\) is defined as

\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) d(v)}},
\]

In topological graph theory, graphs that contain a vertex whose removal yields a planar graphs play an important role, these graphs are called apex graphs [1, 11]. Along these lines a graph \(G\) is called an apex tree [10] if it contains a vertex \(x\) such that \(G - x\) is a tree. The vertex \(x\) is called apex vertex of \(G\). Note that a tree is always an apex tree, hence a non-trivial apex tree is an apex tree which itself is not a tree. For any integer \(k \geq 1\) the graph \(G\) is called \(k\)-apex tree if there exists a subset \(X\) of \(V(G)\) of cardinality \(k\) such that \(G - X\) is a tree and for any \(Y \subset V(G)\) and \(|Y| < k\), \(G - Y\) is not a tree. A vertex in \(X\) is called \(k\)-apex vertex. Clearly, 1-apex trees are precisely non-trivial apex trees. Apex trees and \(k\)-apex trees were introduced in [9] under the name quasi-tree graphs and \(k\)-generalized quasi-tree graphs, respectively. J. Gao found the sharp upper bound of Randić index for apex trees and in this paper, we give sharp upper bound on the Randić index of \(k\)-apex trees for \(k \geq 2\).

### 1.1 Non-regularity of \(k\)-apex trees

We need the following upper bound on Randić index to prove our main results.

**Lemma 1** [2] If \(G\) is a connected graph of order \(n\), then

\[
R(G) \leq \frac{n}{2} - \frac{1}{2} \sum_{uv \in E(G)} \left( \frac{1}{\sqrt{d(u)}} - \frac{1}{\sqrt{d(v)}} \right)^2,
\]

**Lemma 2** The following is an increasing function

\[
f(x) = \left( \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{a}} \right)^2
\]

where \(a\) and \(x\) are positive real numbers and \(x > a\).
Lemma 3 \textit{The function } f(x) = \left(\frac{1}{\sqrt{x+1}} - \frac{1}{\sqrt{x}}\right)^2 \textit{for } x > 0 \textit{ is a decreasing function.}

Theorem 1 \textit{If } G \textit{ is a } k\text{-apex (} k \geq 2) \textit{ tree of order } n \geq 4k - 1, \textit{ then } G \textit{ is not regular.}

\textbf{Proof.} Let } X \subset V(G) \text{ such that } |X| = k \text{ and } G - X \text{ is a tree, then }

\[\sum_{v \in V(G - X)} d_{G - X}(v) = 2n - 2k - 2\]

Suppose that } G \text{ is an } m\text{-regular graph. As } k\text{-apex tree (} k \geq 2) \text{ is never two regular and pendant vertex in } G - X \text{ has at most } k + 1 \text{ degree in } G, \text{ therefore } 3 \leq m \leq k + 1. \text{ Further suppose that } l \text{ is the number of edges in } G \text{ whose one end is in the set } V(G - X) \text{ and other is in the set } X, \text{ then }

\[l \leq mk\]

As } G \text{ is } m\text{-regular, therefore } \sum_{v \in V(G - X)} d_G(v) = mn - mk \text{ and hence }

\[l = \sum_{v \in V(G - X)} d_G(v) - \sum_{v \in V(G - X)} d_{G - X}(v) = mn - mk - 2n + 2k + 2\]

As } l \leq mk, \text{ therefore } mn - mk - 2n + 2k - 2 \leq mk \text{ and hence }

\[m \leq \frac{2n - nk - 2}{n - 2k}\]

As } 3 \leq m, \text{ therefore }

\[3 \leq \frac{2n - nk - 2}{n - 2k}\]

\[n \leq 4k - 2\]

Which is contrary to our supposition that } n \geq 4k - 1. \textit{ Hence } G \textit{ is not } m\text{-regular (} 2 \leq m \leq k + 1) \textit{ that is } G \textit{ is not regular.} \quad \Box
2 Extremal k-apex trees for Randić index

Suppose $\tilde{G}_{n}^{k}$ is the set of all $k$-apex ($k \geq 2$) trees of order $n$ ($n \geq 4k - 1$) such that each $H \in \tilde{G}_{n}^{k}$ has vertices of degree two or three only and has only two asymmetric edges. Then

$$R(H) = \frac{n}{2} - \frac{5 - 2\sqrt{6}}{6}$$

The Fig. 1 is an example of a graph in $\tilde{G}_{18}^{4}$.

![4-apex tree of order 18.](image)

**Lemma 4** If $a \geq 2$ is an integer and $x \geq a + 2$, then the function

$$f(x) = \left( \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{a}} \right)^2 - \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2$$

is an increasing and positive function for $x \geq 4$.

**Corollary 1** If $G$ is a $k$-apex tree of order $n \geq 4k - 1$ which has asymmetric edges degrees of whose vertices are not almost equal, then for any $H \in \tilde{G}_{n}^{k}$

$$R(G) < R(H)$$

**Lemma 5** If $x$ is a real number and $x \geq 4$ then

$$f(x) = (x - 1) \left( \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x-1}} \right)^2 - \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2$$

is greater than zero.
Lemma 6 If $x$ is a real number and $x \geq m \geq 4$, then

$$f(x) = (x - 1) \left( \frac{1}{\sqrt{m}} - \frac{1}{\sqrt{m-1}} \right)^2 - \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right)^2$$

is greater than zero.

Corollary 2 If $G$ is a $k$-apex tree of order $n \geq 4k - 1$, which has at least $2m - 2$ ($2 \leq m \leq k + 2$) asymmetric edges, degrees of whose vertices are almost equal then for any $H \in \tilde{G}_k^n$

$$R(G) < R(H)$$

Figure 2: A 2-apex tree having sharp upper bound

Conjecture 1 If $G$ is $k$-apex ($k \geq 2$) of order $n \geq 4k - 1$, then

$$R(G) \leq \frac{n}{2} - \frac{5 - 2\sqrt{6}}{6}$$

and the equality holds if and only if $G \in \tilde{G}_k^n$.

3 Conclusion

The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies. J. Gao found the sharp upper bound for the Randić index of apex trees. We found that for $k$-apex trees ($k \geq 2$) of order $n \geq 4k - 1$ no regular graphs exist and proposed a conjecture for sharp upper bound for Randić index.

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