On some topological upper bounds of the apex trees

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Outline

Abstract

If a graph G turned out to be a planar graph by removal of a vertex (or a set of vertices) of G, then it is called an apex graph. These graphs play a vital role in the chemical graph theory. On the similar way, a k-apex tree T_n^k is a graph which turned out to be a tree after a removal of k vertices such that k is minimum with this property. Here $|V(T_n^k)| = n$, the cardinality of the set of vertices. In this article, we study different topological indices of apex trees. In particular, we provide upper bounds for the geometric-arithmetic index, the atom bond connectivity index, the augmented Zagreb index and the inverse sum index of the apex and k-apex trees. We identity the graphs for which the equalities hold.

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• for any other subset Y of $V(T^k(n))$ with $|y| < k$, $T^k(n) - Y$ is not a tree.

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- $T^k(n) - X$ is a tree with $|X| = k$
- for any other subset Y of $V(T^k(n))$ with $|y| < k$, $T^k(n) - Y$ is not a tree.
- The elements of X are called k-apex vertices. If $k = 1$, $T(n)$ is called apex tree.

k-apex tree

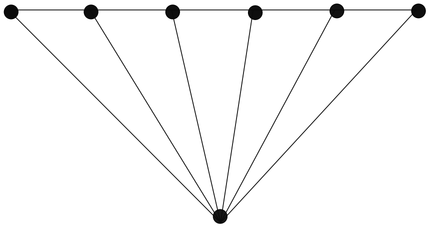

Figure: An apex tree on 7 vertices

k-apex tree

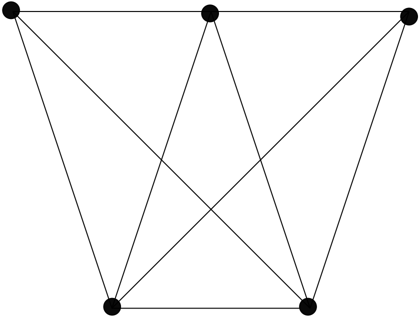

Figure: A 2-apex tree on 5 vertices

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- Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools.
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- Chemical graph theory is branch of Mathematical Chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically.

Topological index

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• A **topological index** is a function

$$Top : \Sigma \longrightarrow R$$

where Σ is the set of finite simple graphs and R is the set of real numbers with property that $Top(G) = Top(H)$ if both G and H are isomorphic.

Wiener Index

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin. He named this index as path number. Later on, path number was renamed as Wiener index and then theory of topological indices started.

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Definition

Let G be a graph. Then the Wiener index of G is defined as $W(G) = \frac{1}{2}\Sigma_{(u;v)}d(u,v)$ where $(u;v)$ is any ordered pair of vertices in G and $d(u;v)$ is $u-v$ geodesic.

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- H. Wiener, J. Amer. Chem. Soc., 69(1947); 17 − −20.

The Zagreb indices

The first Zagreb index M_1 was developed by Gutman and Trinajstiĉ in 1972. This index is significant in the sense that it has many chemical properties and so it attracted many chemists and mathematicians.

Definition

The M_1 index of G is defined as:

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$$

.

The Zagreb indices

The first Zagreb coindex $\overline{M_1}$ was introduced by Došlić.

Definition

The $\overline{M_1}$ of G is defined as $\overline{M_1}(G)$:

$$\overline{M_1}(G) = \sum_{u,v \notin E(G)_{u \neq v}} (d_G(u) + d_G(v))$$

.

The Randić and GA index

Definition

The *Randić connectivity index* of G is given as:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}}.$$

Thus clearly value of $R(G)$ depends upon the degrees of the vertices connected with edges. Later Vukičević and Furtula introduced a topological index named as the *geometric-arithmetic index* (GA index). It is also about the degrees of the vertices connected with edges defined by:

$$\mathrm{GA}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u) d_G(v)}}{d_G(u) + d_G(v)}.$$

The atom-bond connectivity index

In 1998 E. Estrada et al. , introduced the *atom-bond connectivity index* known as the ABC index. The ABC index is very effective topological invariant used to study alkanes energies. The ABC index is some how improvement of the connectivity index χ given by Milan Randi.

Definition

The ABC index is given by:

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}.$$

The augmented Zagreb index

Later Furtula et al. further improved the ABC index and named it as the *augmented Zagreb index* (AZI). In the study of alkanes and octanes energies it was proved that the AZI index performed much better than the ABC index.

Definition

The AZI index is defined as:

$$\mathrm{AZI}(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u)d_G(v)}{d_G(u) + d_G(v) - 2}\right)^3.$$

The inverse sum indeg index

In [?], to estimate the total surface are of octane isomers a new topological index, known as the *inverse sum indeg index* (ISI), is used.

Definition

The ISI has comparatively simple structure and is defined as:

$$\mathrm{ISI}(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_G(u)} + \frac{1}{d_G(v)}} = \sum_{uv \in E(G)} \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v)}.$$

The degree distance index

Dobrynin and Kochetova introduced the degree distance index DD. This index is a weighted version of Wiener index.

Definition

The degree distance index is defined as:

$$DD(G) = \sum_{uv \subset E(G)} d_G(u,v)(d_G(u) + d_G(v))$$

.

In this section we compute upper bounds for the geometric-arithmetic index (GA), the atom-bond connectivity index (ABC), the augmented Zagreb index (AZI), the inverse sum indeg index (ISI) and the degree distance index (DD) of k-apex trees. Note that T_3 is cycle of length 3, so we only consider T_n for $n \geq 4$.

Abstract

Theorem

Let $G \in T(n)$ be an apex tree on n vertices. If $n \geq 4$, then

$$\mathrm{ABC}(G) < \sqrt{\frac{n(n-1)}{3}}$$

Theorem

Let $G \in T^2(n)$ be 2-apex tree on n vertices. If $n \geq 5$, then

$$\mathrm{ABC}(G) \leq \frac{\sqrt{2n-4}}{n-1} + \frac{1}{\sqrt{n-1}}\left(\frac{4}{\sqrt{3}}\sqrt{n} + (n-4)\sqrt{n+1}\right) + \frac{\sqrt{6}}{4}(n-5) + \sqrt{\frac{5}{3}}$$

and the equality holds if and only if $G = K_2 + P_{n-2}$.

Theorem

Let $G \in T^2(n)$ be 2-apex tree on n vertices. If $n \geq 5$, then

$$\begin{aligned} \mathrm{ABC}(G) \leq\ & 3(k-2)\frac{\sqrt{2n-4}}{n-1} + 2k\sqrt{\frac{n+k-2}{(n-1)(k+1)}} + \\ & k(n-k-2)\sqrt{\frac{n+k-1}{(n-1)(k+2)}} + 2\sqrt{\frac{2k+1}{(k+1)(k+2)}} \\ & +(n-k-3)\frac{\sqrt{2k+2}}{k+2}. \end{aligned}$$

and the equality holds if and only if $G = K_k + P_{n-k}$.

Abstract

Theorem

Let $G \in T(n)$ be apex tree on n vertices. If $n \geq 4$, then

$$\mathrm{AZI}(G) \leq 27(n-3)(\frac{n-1}{n})^3 + \frac{729}{64}(n-4) + 32$$

and the equality holds if and only if $G = K_1 + P_{n-1}$.

Theorem

Let $G \in T^2(n)$ be 2-apex tree on n vertices. If $n \geq 5$, then

$$\begin{aligned} \mathrm{AZI}(G) \;\leq\; & \frac{1}{8}\frac{(n-1)^6}{(n-2)^3} + 108\left(\frac{n-1}{n}\right) + \\ & \frac{512}{27}(n-5) + 128(n-4)\left(\frac{n-1}{n+1}\right) \end{aligned}$$

and the equality holds if and only if $G = K_2 + P_{n-2}$.

Theorem

Let $G \in T^k(n)$ be k-apex tree on n vertices. If $k \geq 3$, and $n \geq k+3$, then

$$\begin{aligned} \mathrm{AZI}(G) \;\; \leq \;\; & \frac{3(k-2)(n-1)^6}{8(n-2)^3} + 2k\left(\frac{(n-1)(k+1)}{n+k-2}\right) + \\ & k(n-k-2)\left(\frac{(n-1)(k+2)}{n+k-1}\right) + 2\left(\frac{k^2+3k+2}{2k+1}\right) \\ & + \frac{(n-k-3)(k+2)^6}{8(k+1)^3}. \end{aligned}$$

and the equality holds if and only if $G = K_k + P_{n-k}$.

Abstract

Lemma

If G is a simple connected graph with two non-adjacent vertices u and v, then the following inequality holds.

$$\mathrm{GA}(G + uv) > \mathrm{GA}(G)$$

Theorem

Let $G \in T(n)$ be apex tree on n vertices. If $n \geq 4$, then

$$\mathrm{GA}(G) \leq 2\sqrt{n-1}\left(\frac{2\sqrt{2}}{n+1} + \frac{\sqrt{3}(n-3)}{n+2}\right) + \frac{5n+4\sqrt{6}-20}{5}$$

and the equality holds if and only if $G = K_1 + P_{n-1}$.

Theorem

Let $G \in T^2(n)$ be 2-apex tree on n vertices. If $n \geq 5$, then

$$\mathrm{GA}(G) \leq 1 + \frac{8\sqrt{3(n-1)}}{n+2} + \frac{4(n-4)\sqrt{4(n-1)}}{n+3} + n + \frac{8}{7}\sqrt{3} - 5$$

and equality holds if and only if $G = K_2 + P_{n-2}$.

Theorem

Let $G \in T^k(n)$ be k-apex tree on n vertices. If $k \geq 3$, and $n \geq k+3$, then

$$\begin{aligned} \mathrm{GA}(G) \quad \leq \quad & 3(k-2) + \frac{4k\sqrt{(n-1)(k+1)}}{n+k} + \\ & \frac{2k(n-k-2)\sqrt{(n-1)(k+2)}}{n+k+1} + \\ & \frac{4\sqrt{k^2+3k+2}}{2k+3} + n - k - 3 \end{aligned}$$

and equality holds if and only if $G = K_k + P_{n-k}$.

Abstract

Theorem

Let $G \in T(n)$ be apex tree on n vertices. If $n \geq 4$, then

$$\mathrm{ISI}(G) \leq 4(1 - \frac{2}{n+1}) + \frac{3}{2}(n-4) + 3(n + \frac{15}{n+2} - 6) + \frac{12}{5}$$

and the equality holds if and only if $G = K_1 + P_{n-1}$.

Theorem

Let $G \in T^2(n)$ be 2-apex tree on n vertices. If $n \geq 5$, then

$$\mathrm{ISI}(G) \leq \frac{8(n-4)(n-1)}{n+3} + \frac{12(n-1)}{n+2} + \frac{5}{2}n - \frac{99}{14}$$

and the equality holds if and only if $G = K_2 + P_{n-2}$.

Theorem

Let $G \in T_n^k$ be k-apex tree on n vertices. If $k \geq 3$, and $n \geq k+3$, then

$$\mathrm{ISI}(G) \leq \frac{3}{2}(nk-k-2n) - \frac{1}{4k+6} + \frac{(n-k-3)(k+2)}{2} + \frac{2k(n-1)(k+1)}{n+k} + \frac{k(n-1)(k+2)(n-k-2)}{n+k+1} + \frac{9}{2}$$

and the equality holds if and only if $G = K_k + P_{n-k}$.

Abstract

Lemma

Let $G \in T(n)$ with an apex vertex u and maximum DD. Then

1. $\delta(G) = 2$
2. $d_G(u) = n - 1.$

Lemma

Let G_1 and G_2 be graphs with $|V(G_1)| = n_1$ and $|V(G_2)| = n_2$. Then

$$\begin{aligned} \mathrm{DD}(G_1 + G_2) &= M_1(G_1) + M_1(G_2) + 2(\overline{M_1}(G_1) + \overline{M_1}(G_2)) - \quad (1) \\ &= 2n_2|E(G_1)| - 2n_1|E(G_2)| + n_1 n_2(3n_1 + 3n_2 - 4) \quad (2) \\ &= n_2 \sum_{a \in V(G_1)} d_{G_1}(a) + n_1 \sum_{b \in V(G_2)} d_{G_2}(b). \quad (3) \end{aligned}$$

Theorem

Let $G \in T(n)$ be an apex tree. If $n \geq 4$, then

$$\mathrm{DD}(G) \leq 4n^2 - 10n + 6 + 2\overline{M_1}(T_{n-1}).$$

with equality holding if and only if $G = S_{n-1} + K_1$.

Theorem

Let $G \in T^k(n)$ be a k-apex tree of order n for $k \geq 2$. If $n \geq k+2$, then

$$\mathrm{DD}(G) \leq 3nk(n-k-2) + n(n-1) + 6k^2 + 2\overline{M_1}(T(n-k))$$

with equality holding if and only if $G = S_{n-k} + K_k$.

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Thank You