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Taekyun Kim α-Index of Graphs

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ABSTRACT: In this study, we introduce the Taekyun Kim α-index, a novel topological index for graphs, where $\alpha \in \mathbb{R}$, which involves stresses and degrees of nodes. We calculate this index for a few common graphs and prove a few results. Further, a QSPR analysis is carried for Taekyun Kim 2-index and physical properties of lower alkanes and linear regression models have been provided.

Key Words: Graph, Neighborhood of a node, Stress of a node, Path, Geodesic, Topological index.

Contents

1. Introduction

For common terms and concepts in graph theory, we refer to Harary [2]'s textbook. The unconventional ideas will be provided when needed.

Let $G = (V, E)$ be a undirected graph that is finite and connected. If v is an internal node of a shortest path (also called geodesic) P in G, then we say that P passes through v. The symbol $\deg(v)$ indicates a node v's degree in G.

In 1953, Shimbel presented the idea of a node's stress in a network (graph) as a centrality metric [27]. Numerous fields, including psychology, sociology, and biology, have used this centrality metric (see, for example, [5,25]). The number of geodesics that travel through a node v in a graph G is its stress, and it is represented as $\text{str}_G(v)$ or, in short, by $\text{str}(v)$ if there is no chance of misunderstanding. We designate Θ_G as the highest stress among all of the nodes in G and θ_G as the smallest stress among all of the nodes in G.

K. Bhargava et al. have examined the ideas of total stress of a graph and stress regular graphs in their study [1]. A graph G is k-stress regular if $\text{str}(v) = k$, $\forall v \in V(G)$. The total stress of a graph G, denoted by $N_{\text{str}}(G)$, is defined as

$$N_{\text{str}}(G) = \sum_{v \in V} \text{str}(v).$$

Raksha Poojary et al. [10,11] have studied the concept of total stress of G but by calling it as the stress of G.

A topological index (or connectivity index) of a chemical structure (molecular graph) is nothing but a (real) number that correlates given chemical structure with a physical property or chemical reactivity. Several topological indices have been explored for graphs with numerous applications in Chemistry [29,30], for instance, Wiener index, Harary index, Zagreb index etc.

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R. Rajendra et al. [14] introduced the stress-sum index which is a stress based topological index. The stress-sum index of G, denoted by $\mathcal{SS}(G)$, is defined as

$$\mathcal{SS}(G) = \sum_{uv \in E(G)} [\mathrm{str}(u) + \mathrm{str}(v)] \tag{1.1}$$

C. N. Harshavardhana et al. have conducted a QSPR study for the Stress-Sum Index in [3]. They have shown that the stress-sum index may be used to predict some physical properties of low alkanes.

In their QSPR analysis, R. Rajendra et al. [24] demonstrated that the total stress index is a useful topological index for predicting some physical properties of low alkanes. For new stress/degree based topological indices, we suggest the reader to refer the papers [4,6,7,9,12-24,26,28].

In this work, a finite simple connected graph is referred to as a graph, G denotes a graph and $\mathcal{N}$ denotes the number of geodesics of length ≥ 2 in G. In section 2, a novel topological index for graphs, namely, Taekyun Kim α-index has been introduced, which involves stresses and degrees of nodes. We observe that for $\alpha = 0, 1$, the Taekyun Kim α-index is respectively, the total stress index and stress-sum index. In section 3, some inequalities are established, some results are proved and Taekyun Kim α-index is computed for some standard graphs. In section 4, linear regression models are provided, together with a QSPR analysis for Taekyun Kim 2-index of chemical structures (molecular graphs) and physical properties of lower alkanes.

2. Taekyun Kim α-Index

Definition 2.1 *For a graph $G = (V, E)$, the Taekyun Kim α-index $\mathcal{TK}_\alpha(G)$ is defined by*

$$\mathcal{TK}_\alpha(G) = \sum_{x \in V(G)} str(x) \cdot \deg(x)^\alpha \tag{2.1}$$

where $\alpha \in \mathbb{R}$.

Observation. By Definition 2.1, we have, for any graph $G = (V, E)$,

$$\mathcal{TK}_0(G) = \sum_{v \in V(G)} \mathrm{str}(v) = N_{\mathrm{str}}(G), \text{ the total stress index of } G \text{ (See [1,24])}$$

and

$$\begin{aligned} \mathcal{TK}_1(G) &= \sum_{x \in V(G)} \mathrm{str}(x) \cdot \deg(x) \\ &= \sum_{xy \in E(G)} [\mathrm{str}(x) + \mathrm{str}(y)] \\ &= \mathcal{SS}(G), \text{ the stress-sum index of } G \text{ (See [14]).} \end{aligned}$$

3. Some results

Proposition 3.1 *Let G be a graph. For $\alpha \geq 0$, we have the inequalities:*

$$0 \leq \mathcal{TK}_\alpha(G) \leq |V| \mathcal{N} \Delta_G^\alpha \tag{3.1}$$

and

$$|V| \delta_G^\alpha \theta_G \leq \mathcal{TK}_\alpha(G) \leq |V| \Delta_G^\alpha \Theta_G. \tag{3.2}$$

Proof: For any node v in G, we have $1 \leq \deg(v) \leq \Delta_G$ which implies $1 \leq \deg(v)^\alpha \leq \Delta_G^\alpha$, for $\alpha \geq 0$. Also, for any node v in G, we have $0 \leq \mathrm{str}(v) \leq \mathcal{N}$. Hence

$$0 \leq \mathrm{str}(v) \deg(v)^\alpha \leq \mathcal{N} \Delta_G^\alpha$$

and so by Definition 2.1, the inequality (3.1) follows. For any node v in G, we have $\delta_G \leq \deg(v) \leq \Delta_G$ and $\theta_G \leq \mathrm{str}(v) \leq \Theta_G$. Using these inequalities in Definition 2.1, we establish (3.2). □

Corollary 3.0A *If $\mathcal{N} = 0$ in a graph G, then $\mathcal{TK}_\alpha(G) = 0$. In particular, for a complete graph K_n, $\mathcal{TK}_\alpha(K_n) = 0$.*

Proof: By the Proposition 3.1, it follows that, if $\mathcal{N} = 0$, then $\mathcal{TK}_\alpha(G) = 0$. For K_n, $N = 0$ as there is no geodesic of length ≥ 2, and consequently, $\mathcal{TK}_\alpha(K_n) = 0$. □

Theorem 3.1 *Let G be a graph. Then, $\mathcal{TK}_\alpha(G) = 0$ iff G is a complete graph.*

Proof: Suppose that $\mathcal{TK}_\alpha(G) = 0$. Then it is clear from the Definition 2.1(Eq.(2.1)) that $\mathrm{str}(x) \cdot \deg(x)^\alpha = 0$, $\forall x \in V(G)$. Since G is connected, $\deg(x) \neq 0$ and hence $\mathrm{str}(x) = 0$, for all $x \in V(G)$. If $|V(G)| = 1$ or 2, then G is a complete graph as $G \cong K_1$ or K_2. Assume that $|V(G)| > 2$. Let u, v be any two distinct nodes in G. We claim that u, v are adjacent in G. For, if u, v are not adjacent in G, then there is a geodesic in G between u and v passing through at least one node, say w making $\mathrm{str}(w) \geq 1$, which a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 3.0A, $\mathcal{TK}_\alpha(G) = 0$. □

Proposition 3.2 *For the complete bipartite graph $K_{m,n}$,*

$$\mathcal{TK}_\alpha(K_{m,n}) = \frac{mn\left[n^\alpha(n-1) + m^\alpha(m-1)\right]}{2}.$$

Proof:

Let the partite sets of the complete bipartite graph $K_{m,n}$ be $V_1 = \{v_1, \ldots, v_m\}$ and $V_2 = \{u_1, \ldots, u_n\}$. We have,

$$\mathrm{str}(v_i) = \frac{1}{2}n(n-1) \quad \text{and} \quad \deg(v_i) = n, \quad \text{for } 1 \leq i \leq m \tag{3.3}$$

and

$$\mathrm{str}(u_j) = \frac{1}{2}m(m-1) \quad \text{and} \quad \deg(u_j) = m, \quad \text{for } 1 \leq j \leq n. \tag{3.4}$$

Employing (3.3) and (3.4) in Definition 2.1, we have

$$\begin{aligned}
\mathcal{TK}_\alpha(K_{m,n}) &= \sum_{i=1}^{m} \mathrm{str}(v_i)\deg(v_i)^\alpha + \sum_{j=1}^{n} \mathrm{str}(u_j)\deg(u_j)^\alpha \\
&= \sum_{j=1}^{m}\left[\frac{n(n-1)}{2}n^\alpha\right] + \sum_{i=1}^{n}\left[\frac{m(m-1)}{2}m^\alpha\right] \\
&= \frac{mn^{\alpha+1}(n-1)}{2} + \frac{nm^{\alpha+1}(m-1)}{2} \\
&= \frac{mn\left[n^\alpha(n-1) + m^\alpha(m-1)\right]}{2}.
\end{aligned}$$

□

Proposition 3.3 *If $G = (V, E)$ is an l-regular graph as well as k-stress regular, then*

$$\mathcal{TK}_\alpha(G) = |V|kl^\alpha.$$

Proof: Suppose that G is an l-regular graph as well as k-stress regular. Then

$$\deg(x) = l \text{ and } \mathrm{str}(x) = k, \quad \forall x \in V(G).$$

Using this fact in Definition 2.1, we have

$$\mathcal{TK}_\alpha(G) = \sum_{x \in V(G)} kl^\alpha = |V|kl^\alpha.$$

□

Corollary 3.1B *For a cycle C_n,*

$$\mathcal{TK}_\alpha(C_n) = \begin{cases} n(n-1)(n-3)2^{\alpha-3}, & \text{when } n \text{ is odd;} \\ n^2(n-2))2^{\alpha-3}, & \text{when } n \text{ is even.} \end{cases}$$

Proof: We notice that C_n is a 2-regular graph and for any node v in C_n, we have

$$\text{str}(v) = \begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{when } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}, & \text{when } n \text{ is even.} \end{cases}$$

Therefore, the cycle C_n is

$$\begin{cases} \dfrac{(n-1)(n-3)}{8}\text{-stress regular}, & \text{when } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}\text{-stress regular}, & \text{when } n \text{ is even,} \end{cases}$$

and so by Proposition 3.3, the result follows. □

Proposition 3.4 *Let T be a tree on n nodes. Then*

$$\mathcal{TK}_\alpha(T) = \sum_{v\in I}\left[\sum_{1\le i<j\le m} |C_i^v||C_j^v|\right] m^\alpha,$$

where I is the collection of all internal (non-pendant) nodes in T and the collections $C_1^v, \dots, C_m^v$ denote the node sets of the components of $T - v$ for an internal node v of degree $m = m(v)$.

Proof: Since a pendant node in T has 0 stress, we concentrate on internal nodes and to compute the Taekyun Kim index. Let v be an internal node of T of degree $m = m(v)$. Let $C_1^v, \dots, C_m^v$ be the node sets of the components of $T - v$. As there is only one path between any two nodes in a tree, it is clear that

$$\text{str}(v) = \sum_{1\le i<j\le m} |C_i^v||C_j^v|.$$

Hence by the Definition 2.1, we have

$$\mathcal{TK}_\alpha(T) = \sum_{v\in I}\left[\sum_{1\le i<j\le m} |C_i^v||C_j^v|\right] m^\alpha.$$

where I is the collection of all internal (non-pendant) nodes in T. □

Corollary 3.1C *For path graph P_n on n nodes*

$$\mathcal{TK}_\alpha(P_n) = \frac{2^{\alpha-1}}{3} n(n-1)(n-2).$$

Proof:

Let P_n be the path graph on n nodes (shown in Figure 1) with node set $\{v_1, v_2, \dots, v_n\}$.

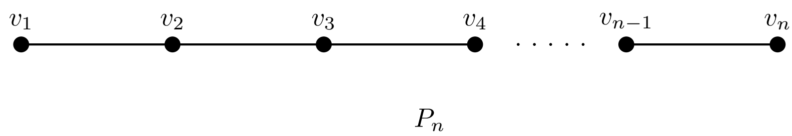

Figure 1: The path P_n on n nodes

We have, $\deg(v_i) = 2$, for $2 \le i \le n-1$ and

$$\mathrm{str}(v_i) = \sum_{1 \le i < j \le 2} |C_i^{v_i}||C_j^{v_i}| = (i-1)(n-i), \text{ for } 2 \le i \le n-1.$$

Therefore, by Proposition 3.4, we have

$$\begin{aligned} \mathcal{TK}_\alpha(T) &= \sum_{i=2}^{n-1} (i-1)(n-i) \cdot 2^\alpha \\ &= 2^\alpha \sum_{i=2}^{n-1} (i-1)(n-i) \\ &= \frac{2^{\alpha-1}}{3} n(n-1)(n-2). \end{aligned}$$ □

Let $Wd(n,m)$ denotes the windmill graph constructed for $n \ge 2$ and $m \ge 2$ by joining m copies of the complete graph K_n at a shared common node v.

Proposition 3.5 *For the windmill graph $Wd(n,m)$,*

$$\mathcal{TK}_\alpha(Wd(n,m)) = \frac{m^{\alpha+1}(m-1)(n-1)^{\alpha+2}}{2}.$$

Hence, for the friendship graph F_k on $2k+1$ nodes, we obtain

$$\mathcal{TK}_\alpha(F_k) = (2k)^{\alpha+1}(k-1).$$

Proof: Any node other than the universal node has 0 stress in $Wd(n,m)$. The only geodesics passing through universal node v are of length 2. So, $\mathrm{str}(v) = \frac{m(m-1)(n-1)^2}{2}$. Note that $\deg(v) = m(n-1)$. So, by Definition 2.1, we have

$$\begin{aligned} \mathcal{TK}_\alpha(Wd(n,m)) &= \frac{m(m-1)(n-1)^2}{2} \cdot [m(n-1)]^\alpha \\ &= \frac{m^{\alpha+1}(m-1)(n-1)^{\alpha+2}}{2}. \end{aligned}$$

As the friendship graph F_k on $2k+1$ nodes is the windmill $Wd(3,k)$, we have

$$\mathcal{TK}_\alpha(F_k) = \frac{k^{\alpha+1}(k-1)(3-1)^{\alpha+2}}{2} = (2k)^{\alpha+1}(k-1).$$ □

Proposition 3.6 *Let W_n denote the wheel graph on $n \ge 4$ nodes. Then*

$$\mathcal{TK}_\alpha(W_n) = \begin{cases} \dfrac{(n-1)^{\alpha+1}(n-4)}{2} + \dfrac{3^\alpha(n-1)(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^{\alpha+1}(n-4)}{2} + \dfrac{3^\alpha(n-1)^2(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases}$$

Proof: In W_n with $n \geq 4$, there are $n-1$ peripheral nodes and one central node, say v. Then

$$\text{str}(v) = \frac{(n-1)(n-4)}{2}. \tag{3.5}$$

Let q be a peripheral node. Note that v is adjacent to all the peripheral nodes in W_n. So, there is no geodesic passing through q containing v. Hence contributing nodes for $\text{str}(q)$ are the remaining peripheral nodes. Let us denote the cycle $W_n - v$ (on $n-1$ nodes) by C_{n-1}. Then

$$\begin{aligned}\text{str}_{W_n}(q) &= \text{str}_{W_n - v}(q)\\ &= \text{str}_{C_{n-1}}(q)\\ &= \begin{cases}\dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;}\\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,}\end{cases}\\ &= \begin{cases}\dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;}\\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.}\end{cases}\end{aligned} \tag{3.6}$$

Let us denote the set of all the peripheral nodes in W_n by P. Then, using (3.5) and (3.6) in the Definition 2.1, we have

$$\begin{aligned}\mathcal{TK}_\alpha(W_n) &= \text{str}(v)\deg(v)^\alpha + \sum_{q \in P} \text{str}(q)\deg(q)^\alpha\\ &= \frac{(n-1)(n-4)}{2}\cdot(n-1)^\alpha + 3^\alpha(n-1) \times \begin{cases}\dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;}\\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.}\end{cases}\\ &= \begin{cases}\dfrac{(n-1)^{\alpha+1}(n-4)}{2} + \dfrac{3^\alpha(n-1)(n-2)(n-4)}{8}, & \text{if } n \text{ is even;}\\ \dfrac{(n-1)^{\alpha+1}(n-4)}{2} + \dfrac{3^\alpha(n-1)^2(n-3)}{8}, & \text{if } n \text{ is odd.}\end{cases}\end{aligned}$$

□

4. QSPR Analysis for Taekyun Kim α-index when $\alpha = 2$

As we observed in section 2, Taekyun Kim 0-index and Taekyun Kim 1-index are respectively, total stress index and stress-sum Index. After conducting a QSPR analysis for the total stress index, R. Rajendra et al. [24] have demonstrated that the total stress is a helpful topological index for predicting the physical properties of low alkanes, such as boiling points, molar volumes, molar refractions, heats of vaporisation, critical temperatures, and critical pressures. C. N. Harshavardhana et al. have conducted a QSPR analysis for the Stress-Sum Index in [3], and they showed that the stress-sum index can be used to predict the boiling points, molar volumes, molar refractions, heats of vaporisation, and critical temperatures of low alkanes.

In this section, a QSPR analysis is carried for Taekyun Kim 2-index of chemical structures (molecular graphs) and physical properties of lower alkanes and linear regression models are presented.

The experimental values for the physical properties - Boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions(st) $dyne\ cm^{-1}$ of considered alkanes are given in Table 1 along with the Taekyun Kim 2-index of chemical structures (molecular graphs). The numerical values in columns 3 to 9 of the Table 1 are obtained from [30] (the same can be referred in [8]).

Table 1: Taekyun Kim 2-index and values of the physical properties of considered low alkanes

Alkane	$\mathcal{TK}_2$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	40	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	57	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	96	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	80	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	103	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	104	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	160	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	126	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	140	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	169	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	171	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylpentane	168	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	244	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	200	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	198	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	248	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	273	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	224	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	259	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	262	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	263	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	256	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	352	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	298	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	297	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	294	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	360	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	300	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	291	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	360	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	363	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	339	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	459	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	333	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	336	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	377	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	381	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	383	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	372	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	324	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	488	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	424	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	424	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	422	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	418	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	500	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	428	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	426	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	504	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	410	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	413	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	500	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	417	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	535	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	533	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	529	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	545	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	469	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	465	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	541	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	545	140.5	172.1	43.34	42.3	330.6	26.45	23.27

3,3-Diethylpentane	496	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	524	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	513	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	451	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	652	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	540	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	640	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	586	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models

An investigation was conducted with a linear regression model

$$P = A + B \cdot \mathcal{TK}_2$$

where P = Physical property and $\mathcal{TK}_2$ =Taekyun Kim 2-index, using Table 1.

The computed values of correlation coefficient r, its square r^2, standard error (se), t-value and p-value are presented in Table 2 followed by the linear regression models.

Table 2: r,r^2, se, t and p for the physical properties (P) and $\mathcal{TK}_2$ stress

P	r	r^2	se		t		p	
bp	0.8111	0.6579	(5.8659)	(0.0152)	(9.8250)	(10.7019)	$(1.52599E-14)$	$(4.61791E-16)$
mv	0.8542	0.7297	(2.8429)	(0.0073)	(45.6139)	(12.7871)	$(1.24185E-51)$	$(1.58524E-19)$
mr	0.8819	0.7778	(0.7847)	(0.0020)	(37.0404)	(14.6281)	$(6.90904E-46)$	$(2.17078E-22)$
hv	0.7477	0.5590	(1.1482)	(0.0030)	(25.9433)	(8.6413)	$(2.44835E-36)$	$(1.89108E-12)$
ct	0.8453	0.7145	(6.5195)	(0.0169)	(33.5375)	(12.2580)	$(3.50939E-43)$	$(1.14183E-18)$
cp	-0.6580	0.4330	(0.6271)	(0.0016)	(47.8593)	(-6.5749)	$(5.70924E-53)$	$(9.16994E-09)$
st	0.7364	0.5423	(0.4513)	(0.0011)	(40.0614)	(7.2315)	$(1.54655E-46)$	$(7.88566E-10)$

For boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes, the linear regression models are given below:

$$bp = 57.63236563 + 0.162294077 \cdot \mathcal{TK}_\alpha \tag{4.1}$$

$$mv = 129.6741969 + 0.09397958 \cdot \mathcal{TK}_\alpha \tag{4.2}$$

$$mr = 29.06511531 + 0.029674939 \cdot \mathcal{TK}_\alpha \tag{4.3}$$

$$hv = 29.78817922 + 0.025650867 \cdot \mathcal{TK}_\alpha \tag{4.4}$$

$$ct = 218.6475042 + 0.206604389 \cdot \mathcal{TK}_\alpha \tag{4.5}$$

$$cp = 30.01382183 - 0.010659737 \cdot \mathcal{TK}_\alpha \tag{4.6}$$

$$st = 18.07785152 + 0.008255737 \cdot \mathcal{TK}_\alpha \tag{4.7}$$

From the Table 2, it follows that the linear regression models (4.1)-(4.5) can be used to make predictions.

Conclusion

In this paper, a novel topological index for graphs has been introduced, namely, Taekyun Kim α-index which involves stresses and degrees of nodes, where $\alpha \in \mathbb{R}$. For $\alpha = 0, 1, 2$, it is observed that Taekyun Kim α-index can be used as a predictive measure for physical properties of low alkanes. It will be interesting to explore the properties of Taekyun Kim α-index for various real values of α.

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