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TRANSIT INDEX OF A GRAPH AND ITS CORRELATION WITH MON OF OCTANE ISOMERS

K. M. RESHMI[1] AND RAJI PILAKKAT

ABSTRACT. Many topological indices are defined for Graphs. Some are distance based and some are degree based. Topological indices are widely used to analyse various networks, from large complex networks in communications to molecular graphs in chemical graph theory. In this paper we define new graph parameters called transit of a vertex and transit index of a graph. We compute them for Paths and Trees. It is found that among all trees on n vertices, the path P_n has the maximum transit index. The bounds for transit index are determined for connected graphs. Finally, the correlation coefficient between transit index of molecular graphs of octane isomers and motor octane number is evaluated. The correlation coefficient obtained is strongly negative

1. INTRODUCTION

Graph theory is a branch of Mathematics that finds application in various fields of science and technology. Graph topologies are extensively studied in Chemical graph Theory and Computer Networking. The concept of topological indices owes to Weiner [8], [9]. He introduced it while studying the boiling point of paraffins. Hyper-Weiner index [5] and Schultz index [6] are also distance based topological indices, while Randić [3] index and Zagreb index [1] are degree based. Structural properties of graphs were also studied in various communication networks. Many graph invariants related to centrality gained attention. In the paper [7], Shimbel introduced a graph parameter named "stress

[1]*corresponding author*
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of a vertex". Stress of a vertex v is the number of shortest paths which passes through v. Motivated by this parameter we define the transit of a vertex and transit index of a graph . The degree of vertices and graph distances has its effect on the transit.

Throughout this paper, G denotes a simple, connected and undirected graph with vertex set V and edge set E. Also $|V| = n$ and $|E| = m$. For undefined terms we refer [2].

2. Transit index

Definition 2.1. *Let $v \in V$. Then we define the transit of a vertex v denoted by $T(v)$ as "the sum of the lengths of all shortest path with v as an internal vertex " and the transit index of G denoted by $TI(G)$ as*

$$TI(G) = \sum_{v \in V} T(v)\,.$$

Lemma 2.1. *$T(v) = 0$ iff $\langle N[v] \rangle$ is a clique.*

Proof. Let $T(v) = 0$. Consider the degree $d(v)$ of v. If $d(v) = 0, 1$, then we are done. Let $d(v) > 1$. Let $V_k = \{v_1, v_2, \ldots, v_k\}$ be the neighbours of v. Let us suppose that $\langle N[v] \rangle$ is not a clique. Without loss of generality, let us assume that v_r and v_s are two non-adjacent neighbours of v. In this case v_r, v, v_s forms a shortest path through v. A contradiction to the assumption.

Conversely let $N[v] = V_k \cup \{v\}$ forms a clique.

If $d(v) = 0, 1$, then there are no paths passing through v and hence $T(v) = 0$. Let $d(v) > 1$ and if possible, let $T(v) \neq 0$. Then there exist a shortest path $P : u, \ldots, u_1, v, v_1, \ldots, w$ passing through v. Since u_1, v_1 are neighbours of v,they are adjacent. Hence the $u - w$ path $P - \{v\}$ obtained from P by deleting the vertex v from P forms a $u - w$ path with less length than P, a contradiction. □

3. Paths and Trees

Theorem 3.1. *For a path P_n,*

$$\text{transit index } = \frac{n(n+1)(n^2 - 3n + 2)}{12}$$

Proof. Let $P_n : v_1 v_2 \ldots v_n$. Then v_k divides P_n into two paths say P_1 with $k-1$ vertices and P_2 with $n-k$ vertices.

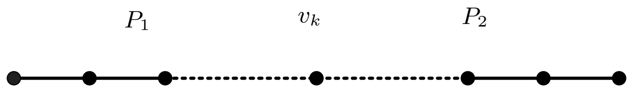

FIGURE 1. Path P_n

We will compute $T(v_k)$ by counting the number of times each edge appears in the shortest path passing through v_k. The edges in P_1 will be used

$$1.(n-k-1), 2.(n-k-1), 3.(n-k-1), \ldots, k.(n-k-1)$$

times respectively and the edges in P_2 will be used

$$1.(k-1), 2.(k-1), 3.(k-1), \ldots, (n-k-1)(k-1)$$

times. Hence

$$\begin{aligned} T(v_k) &= 1.(n-k-1) + 2.(n-k-1) + 3.(n-k-1) + \ldots + k.(n-k-1) \\ &\quad +1.(k-1) + 2.(k-1) + 3.(k-1) + \ldots + (n-k-1)(k-1) \\ &= \frac{(k-1)k(n-k)}{2} + \frac{(n-k+1)(n-k)(k-1)}{2} \\ &= \frac{(k-1)(n-k)[k+n-k+1]}{2} \\ T(v_k) &= \frac{(n+1)(k-1)(n-k)}{2}. \end{aligned}$$

Hence, the transit index ,

$$\begin{aligned} TI(P_n) &= \sum_{k=1}^{n} T(v_k) = \sum_{k=1}^{n} \frac{(n+1)(n-k)(k-1)}{2} \\ &= \frac{n(n+1)(n^2-3n+2)}{12} \end{aligned}$$

$\square$

Theorem 3.2. *Let T be a tree and v be any vertex of T. Let $\{T_j\}$ be the branches of v, with vertex set $\{V_j = \{u_{ij}, i = 1, 2, \ldots\}\}$ and edge set $E_j = \{E(V_j)\} = \{e_{ij}, i = 1, 2, \ldots\}$. Consider v as the root and v_{ij} as vertices below it as shown in the figure. Let $d(e_{ij})$ denote the number of edges below e_{ij}. Then the transit of v is*

$$T(v) = \sum_j \left[(n-1-n_j) \sum_i d(e_{ij}) \right] = \sum_j \left[(n-1-n_j) \sum_i d(v, u_{ij}) \right],$$

where $n_j = |V_j|$.

Proof. To find the transit of a vertex, we find the contribution of each edge to $T(v)$. In every shortest path passing through v, the edges will be used by vertices lying below it to travel to all the vertices in other branches.

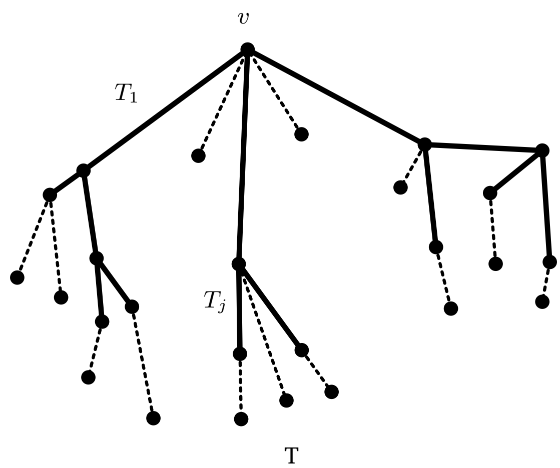

FIGURE 2. Tree rooted at v

Hence the contribution of an edge u_{ij} of T_j is $d(e_{ij})(n-1-n_j)$. Hence contribution of the whole branch T_j will be$(n-1-n_j)\sum_i d(e_{ij})$

$$\therefore T(v) = \sum_j \left[(n-1-n_j) \sum_i d(e_{ij}) \right].$$

Since the contribution of the edges in T_j can also be computed as $\sum_i d(v, u_{ij})$, we have

$$T(v) = \sum_j \left[(n-1-n_j) \sum_i d(v, u_{ij}) \right].$$

$\square$

Remark 3.1. *In a tree,* $T(v) = \sum_j (n-1-n_j)\frac{n_j(n_j+1)}{2}$*, when* v *has all its branches as paths.*

Lemma 3.1. *Let* P_n *be a path on* n *vertices. By adding a pendant vertex, the transit index is maximised if the vertex is added to either of the ends and minimised when it is added to the center vertex of* P_n*.*

Proof. Consider the path P_n. Let us attach a new vertex v to the kth vertex v_k of P_n. Let I denote the increment in transit Index due to this action. i.e. $I = TI(P_n + v) - TI(P_n)$. We will show that I is minimum when $k = \frac{n+1}{2}$

I	$=$	Increment in T(u),$\forall u \in P_n$
For u=k	the increment is	$2+3+\ldots+k+2+3+\ldots+n-k+1$
For u=k-1	$\rightarrow$	$3+4+\ldots+k$
$\vdots$		
$\vdots$		
For u=2		k
For u=1		0
For u=k+1		$3+4+\ldots+n-k+1$
For u=k+2		$4+5+\ldots+n-k+1$
$\vdots$		
$\vdots$		
For u=n-1		$n-k+1$
For u=n		0
$\therefore I$	$=$	$(k-1)k(k+1)+(n-k)(n-k+1)(n-k+2)$

Now if we consider I as a real function of k on the closed interval $[1, n]$, its extrema are either at boundaries or when $\frac{dI}{dk} = 0$.

$$\frac{dI}{dk} = 0 \Longrightarrow k = \frac{n+1}{2}$$

Hence extrema occurs at $k = 1, n, \frac{n+1}{2}$.

k	I(k)
1	(n-1)n(n+1)
n	(n-1)n(n+1)
$\frac{n+1}{2}$	$\frac{(n-1)(n+1)(n+3)}{8}$

Clearly maximum is for $k = 1, n$ and minimum for $k = \frac{n+1}{2}$ □

Lemma 3.2. *Let e be an edge of G. If G and $G - e$ are connected, $TI(G) < TI(G - e)$.*

Proof. Let G be a connected graph. Let $e = uv$ be such that $G - e$ is connected. By removing e, u and v becomes non adjacent. Since $G - e$ is connected there exist some shortest path P connecting u and v of length ≥ 2. This will increase the transit of every internal vertex of P in $G - e$. Hence the proof. □

Remark 3.2. *Among all connected graphs on n vertices, trees have the maximum transit index. (Since trees are the minimal connected graphs on n vertices.)*

Theorem 3.3. *Among all trees on n vertices, the transit index is maximum for the path P_n.*

Proof. Proof by induction on n. The result is trivially true for $n = 2, 3$ as there exist only one tree. For $n = 4$, there are only 2 non isomorphic trees. One is the path P_4 and other is the star S_4. We have $TI(P_4) = 10$ and $TI(S_4) = 6$. Hence true for $n = 4$. For $n = 5$, there are 3 non isomorphic trees, P_5, S_5 and G as shown in the figure. Here $TI(P_5) = 30, TI(S_5) = 12, TI(G) = 14$. Hence true for $n = 5$ also. Let us assume that transit index is maximum for P_n on all trees on $\leq n$ vertices. Let us consider all trees on $n + 1$ vertices. Let the transit index be maximum for some tree T, on $n + 1$ vertices. Let P be a path in T of maximum length. If $P = P_{n+1}$, we are done. If not, let $P = P_k$, $k \leq n$. By induction hypothesis, among all trees on $\leq n$ vertices P_n has maximum transit index. Now, with application inductively on the pendant vertices of P we can show that $P = P_{n+1}$. Hence the proof. □

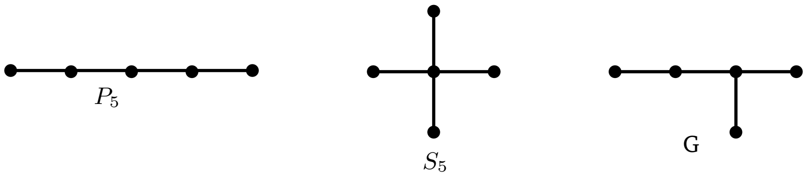

FIGURE 3. Non isomorphic trees on 5 vertices

Remark 3.3. *For a connected graph G on n vertices, $0 \leq TI(G) \leq n(n+1)\frac{(n^2-3n+2)}{12}$. The bounds are attained by K_n and P_n respectively.*

4. CORRELATION BETWEEN MON AND TRANSIT INDEX

Researchers have presented many molecular descriptors/topological indices so far.

Octane Isomer	TI(G)	MON
n-octane	252	-
2-methyl-heptane	212	23.8
3-methyl-heptane	188	35
4-methyl-heptane	180	39
3-ethyl-hexane	156	52.4
2,2-dimethyl-hexane	156	77.4
2,3-dimethyl-hexane	149	78.9
2,4-dimethyl-hexane	152	69.9
2,5-dimethyl-hexane	174	55.7
3,3-dimethyl-hexane	128	83.4
3,4-dimethyl-hexane	132	81.7
2-methyl-3-ethyl-pentane	124	88.1
3-methyl-3-ethyl-pentane	108	88.7
2,2,3-trimethyl-pentane	104	99.9
2,2,4-trimethyl-pentane	122	100
2,3,3-trimethyl-pentane	98	99.4
2,3,4-trimethyl-pentane	114	95.9
2,2,3,3-tetramethylbutane	78	-

TABLE 1. Transit Index and Motor Octane Number of Octane Isomers

Molecular descriptors are useful in structure-property and structure-activity studies. Suggestions about the required characteristics of molecular descriptors are discussed in [4]. A good correlation with at least one physical/chemical property and some discrimination power among isomers are ideal. On investigation it was found that transit index of octane isomers hold a strong negative correlation with MON(motor octane number).

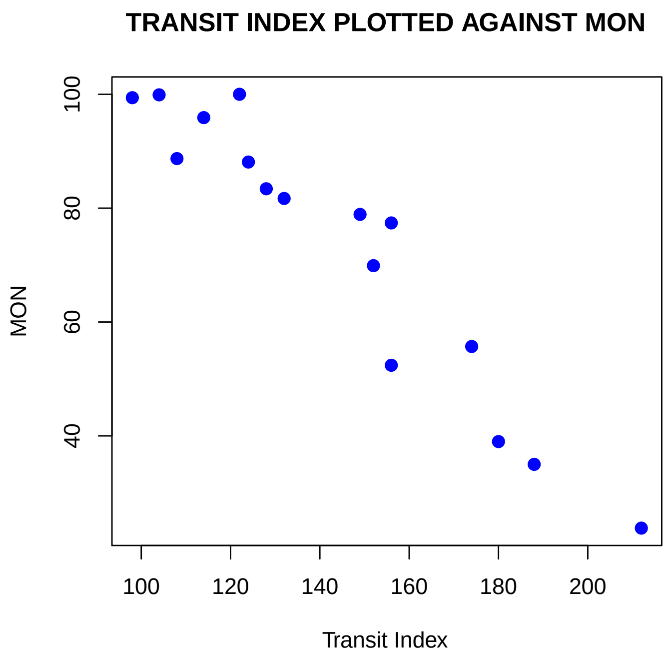

FIGURE 4. Scatter Plot

In Table 1, transit index of octane isomers and MON are presented. Using the table 1, the scatter plot between $TI(G)$ and MON is exhibited in figure 4. The correlation coefficient obtained is **-0.9544**

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DEPARTMENT OF MATHEMATICS
GOVERNMENT ENGINEERING COLLEGE
KOZHIKODE-673005, KERALA, INDIA
E-mail address: reshmikm@gmail.com

DEPARTMENT OF MATHEMATICS
UNIVERSITY OF CALICUT
MALAPPURAM-673365, KERALA, INDIA
E-mail address: rajipilakkat@gmail.com