



Transit index by means of graph decomposition

K.M. Reshmi^{1*} and Raji Pilakkat²

Abstract

Many topological indices for graphs are defined and are widely studied. Some are distance based and some are degree based. They find applications in many fields like chemical graph theory and networking. The concept of transit of a vertex and transit index of a graph was defined by the authors in their previous work. The transit of a vertex v is “the sum of the lengths of all shortest path with v as an internal vertex” and the transit index of G is $TI(G)$ is the sum of the transit of all vertices of G . In this paper we introduce the concept of majorized shortest path, transit decomposition of a graph and transit decomposition number.

Keywords

Transit Index, Majorized shortest path, Transit decomposition, Transit decomposition number.

AMS Subject Classification

05C10, 05C12.

¹Department of Mathematics, Government Engineering College, Kozhikode-673005, Kerala, India.

²Department of Mathematics, University of Calicut, Malappuram-673365, Kerala, India.

*Corresponding author: ¹reshmikm@gmail.com; ²rajipilakkat@gmail.com

Article History: Received 24 October 2020; Accepted 19 December 2020

©2020 MJM.

Contents

1	Introduction	2208
2	Majorized shortest paths	2209
3	Transit decomposition	2210
	References	2211

1. Introduction

In the fields of chemical graph theory, molecular topology and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. In[4], transit index of a graph was introduced and its correlation with one of the physical property -MON of octane isomers was established.

In this paper we introduce the concept of majorized shortest path and transit decomposition of a graph. We also discuss certain results which helps in computing transit index of graphs. The transit decomposition number in case of certain graphs are also determined.

Throughout G denotes a simple, connected, undirected graph with vertex set V and edge set E . For undefined terms we refer [1].

Preliminaries

Definition 1.1. [4] Let v be any vertex of G . Then the transit of v denoted by $T(v)$ is “the sum of the lengths of all shortest path with v as an internal vertex” and the transit index of G denoted by $TI(G)$ is

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

Lemma 1.2. [4] For a vertex v of the graph G , $T(v) = 0$ iff $\langle N[v] \rangle$ is a clique. ie $T(v) = 0$ iff v is a simplicial vertex of G

Theorem 1.3. [4] For a path P_n , Transit index is

$$TI(P_n) = \frac{n(n+1)(n^2-3n+2)}{12}$$

Theorem 1.4. [5] Let C_n be a cycle with n even. Then

$$i) TI(C_n) = \frac{n^2(n^2-4)}{24}$$

$$ii) TI(C_{n+1}) = \frac{n(n^2-4)(n+1)}{24}$$

Definition 1.5. [5] Two vertices v_1 and v_2 of a graph are called **transit identical** if the shortest paths passing through them are same in number and length.

2. Majorized shortest paths

Definition 2.1. A path M through v is called a majorized shortest path of v , abbreviated as $msp(v)$ or msp , if it satisfies the following conditions.

1. M is a shortest path in G with v as an internal vertex.
2. There exists no path M' such that, M' is a shortest path in G with v as an internal vertex and M as a subpath of it.

We denote the collection of all $msp(v)$ by \mathcal{M}_v and $\bigcup_{v \in V} \mathcal{M}_v$ by

\mathcal{M}_G

Example 2.2. Consider the graph G in figure [1]. Let $M_1 : 1234, M_2 : 1235, M_3 : 123$. Then M_1 and M_2 are $msp(2)$, while M_3 is not a majorized shortest path of 2.

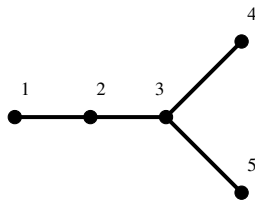


Figure 1. Graph G

\mathcal{M}_G for various graphs

1. For a path P_n , $\mathcal{M}_G = \{P_n\}$
2. For a star S_n , \mathcal{M}_G is the collection of all paths of length 2 connecting two pendant vertex.

We know that there are $C(n-1, 2)$ such paths and their intersection is $\{c\}$, where c is the central vertex

$$\therefore TI(G) = C(n-1, 2) \times TI(P_3) = (n-1)(n-2)$$

3. For a cycle C_n , $n > 3$, every majorized shortest path is d in length, where d is the diameter.

For every vertex $v \in C_n$, $|\mathcal{M}_v| = d - 1$. Hence $|\mathcal{M}_G| = n$.

Proposition 2.3. For a graph G , \mathcal{M}_G is unique.

Proposition 2.4. Let $e = uv$ be any edge of G . If e is not a part of any majorized shortest path in G , then $e \in C_3$

Proof. Let us assume that e is not a part of any majorized shortest path in G . Let $v_1 \neq u$ be a neighbour of v in G . Then the shortest path from v_1 to u is of length ≤ 2 . If it is 2, the path v_1vu will be a part of the majorized shortest path through v . Hence $d(u, v_1) = 1$, showing $e = uv$ is part of C_3 . \square

Proposition 2.5. In a tree T , $msp(v)$ connects pendant vertices of $T, \forall v \in V$. Conversely every path connecting two pendant vertex is a msp for every internal vertex of it.

Proof. Suppose M be a $msp(v), v \in T$. Let $M : v_1v_2 \dots v \dots v_k$. Suppose if possible one of the end vertex of M be a non

pendant vertex of T . Without loss of generality let us assume v_1 is not a pendant vertex. Then $d(v_1) > 1$. Let u be a neighbor of v_1 other than v_2 . Then the path $uv_1v_2 \dots v \dots v_k$ is a shortest path in T with v as an internal vertex and with M as a subpath of it. This is a contradiction.

Conversely, let M be a path connecting two pendant vertices, say u_1 and u_2 of T . Let v be an internal vertex of M . We need to show that $M \in \mathcal{M}_v$. Assume $M \notin \mathcal{M}_v$. Then either (i) M is not a shortest path in T or (ii) M is a subpath of some M' with v as an internal vertex. Since T is a tree, $u_1 - u_2$ path is unique and hence M is a shortest path. So (i) does not hold. Again u_1, u_2 are pendant vertices proves (ii) wrong.

Hence the proof. \square

Corollary 2.6. $|\mathcal{M}_T| = C(p, 2)$, where T is a tree and p the number of pendant vertices of T .

Proposition 2.7. Consider the graph $G(V, E)$. Let $v \in V$ and \mathcal{M}_v be the collection of all majorized paths in G with v as an internal vertex. If $\mathcal{M}_v = \{M_1, M_2\}$, then $T(v) = T_{M_1}(v) + T_{M_2}(v) - T_{M_1 \cap M_2}(v)$

Proof. Given $\{M_1, M_2\} = msp(v)$. Let \mathcal{S} be the collection of all shortest paths in G with v as an internal vertex. Then $T(v) = \text{sum of lengths of paths in } \mathcal{S}$

Let \mathcal{S}_1 and \mathcal{S}_2 be the collection of all subpaths of M_1, M_2 with v as an internal vertex, respectively. Then $T_{M_i}(v)$ is the sum of the lengths of the paths in \mathcal{S}_i .

Consider $M_1 \cap M_2$. Either $M_1 \cap M_2 = \{v\}$ or $M_1 \cap M_2$ is a subpath of M_1 and M_2 with v as an internal vertex. Let \mathcal{S}' be the collection of subpaths of $M_1 \cap M_2$ with v as an internal vertex. Then $\mathcal{S}' \subset \mathcal{S}_1$ and $\mathcal{S}' \subset \mathcal{S}_2$. Hence the proof. \square

Let $G(V, E)$ and \mathcal{M}_v be the collection of all majorized path in G with v as an internal vertex. If $\mathcal{M}_v = \{M_i, i = 1, 2, \dots, k\}$, then the result[2.7] could be extended by applying the inclusion-exclusion principle in set theory.

Theorem 2.8. Let $G(V, E)$ be a graph and $v \in V$. If $\mathcal{M}_v = \{M_1, M_2, \dots, M_k\}$ then, $T(v) = T_{M_1}(v) + \dots + T_{M_k}(v) - T_{M_1 \cap M_2}(v) - \dots - T_{M_{k-1} \cap M_k}(v) + \dots + (-1)^{k+1} T_{M_1 \cap M_2 \cap M_3 \dots \cap M_k}(v)$

Proposition 2.9. Let $G(V, E)$ and \mathcal{M}_G be the collection of all majorized paths in G . If $\mathcal{M}_G = \{M_1, M_2\}$, then $TI(G) = TI(M_1) + TI(M_2) - TI(M_1 \cap M_2)$

Proof.

$$\begin{aligned} TI(G) &= \sum_{v \in V} T(v) \\ &= \sum_{v \in V} [T_{M_1}(v) + T_{M_2}(v) - T_{M_1 \cap M_2}(v)] \\ &= \sum_{v \in M_1} T(v) + \sum_{v \in M_2} T(v) - \sum_{v \in M_1 \cap M_2} T(v) \\ &= TI(M_1) + TI(M_2) - TI(M_1 \cap M_2) \end{aligned}$$

\square



Let $G(V, E)$ be a graph and \mathcal{M}_G be the collection of all majorized path in G . If $\mathcal{M}_G = \{M_i, i = 1, 2, \dots, k\}$, then the result[2.9] could be extended by applying the inclusion-exclusion principle in set theory.

Theorem 2.10. Let $G(V, E)$ be a graph and \mathcal{M}_G be the collection of all majorized path in G . If $\mathcal{M}_G = \{M_i, i = 1, 2, \dots, k\}$, $TI(G) = T_v(M_1) + \dots + T_v(M_k) - T_v(M_1 \cap M_2) - \dots - T_v(M_{k-1} \cap M_k) + \dots + (-1)^{k+1} T_v(M_1 \cap M_2 \cap M_3 \dots \cap M_k)$. Hence knowing the majorized shortest paths of a graph, one could compute the transit index of a graph.

3. Transit decomposition

Definition 3.1. A decomposition of a graph G into a collection of subgraphs $\tau = \{T_1, T_2, \dots, T_r\}$, where each T_i is either a chordless cycle in G or a majorized shortest path of G such that $TI(G) = \sum_i TI(T_i) - \sum_{i \neq j} TI(T_i \cap T_j) + \dots + (-1)^{r+1} \sum TI(T_1 \cap T_2 \cap \dots \cap T_r)$ is called a Transit Decomposition of G . We denote a transit decomposition of minimum cardinality by τ_{min} .

The minimum cardinality of a transit decomposition of G is called the Transit decomposition number, denoted by $\theta(G)$ or simply θ if there is no other confusion. Clearly \mathcal{M}_G is a transit decomposition of G . We denote $|\mathcal{M}_G|$ by $\theta_a(G)$ or simply θ_a .

Example 3.2. Consider the graph in the figure [2]. Let $M_1 : 1234; M_2 : 1254; M_3 : 345; M_4 : 325; C_1 : 23452$. Here

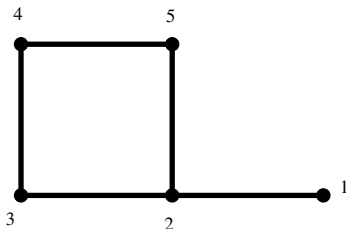


Figure 2. Graph G

$\mathcal{M}_G = \{M_1, M_2, M_3, M_4\}$. Here $\tau_{min} = \{M_1, M_2, C_1\}$, the transit decomposition of minimal cardinality. Hence $\theta = 3$, while $\theta_a = 4$.

Proposition 3.3. If C_n is a chordless cycle in G , with $n > 3$, then $C_n \in \tau_{min}$.

Remark 3.4. If e is an edge of G that does not belong to any cycle in G , it will be a part of some $T_i \in \tau$

Transit decomposition number for various graphs

- If G is a tree, $\tau = \mathcal{M}_G$ and $\theta = \theta_a = C(p, 2)$, where p is the number of pendant vertices.

- If G is a cycle, $\theta = 1$ and $\theta_a = n, n > 3$
- If G is a path, $\theta = \theta_a = 1$.
- If G is a complete graph, $\theta = \theta_a = 0$.

Theorem 3.5. Let $G = K_{p,q}$, the bipartite graph. Then $\theta = \frac{p(p-1)q(q-1)}{4}$ and $\theta_a = \frac{pq(p+q-2)}{2}$.

Proof. In the case of a complete bipartite graphs, every shortest path is of length ≤ 2 . Hence every shortest path is a majorized shortest path. $\therefore \theta_a = \sum_1^q c(p, 2) + \sum_1^p c(q, 2) = \frac{pq(p+q-2)}{2}$

The chordless cycles in $K_{p,q}$ is of girth 4. Also every shortest path is part of some chordless cycle. Hence $\theta =$ the number of cycles in $K_{p,q}$ of girth 4 $= C(p, 2) \times C(q, 2) = \frac{p(p-1)q(q-1)}{4}$ \square

Theorem 3.6. Let $G = W_n, n > 4$, be the wheel graph. Then $\theta = \theta_a = \frac{(n-1)(n-2)}{2}$

Proof. In the wheel graph every chordless cycle is C_3 . Hence $\theta = \theta_a$. Note that the diameter of the graph is 2. Hence every majorized shortest path is of length ≤ 2 . Since P_2 is not a majorized shortest path(msp), all msp in G are isomorphic to P_3 . On the cycle of the wheel, starting with every vertex there are 2 msp. Hence on a total $(n-1)$ paths.

Other msp are those starts and ends on the cycle of the wheel and passes through the center. With each vertex on the cycle we can associate $(n-4)$ such paths. Hence on a total $\frac{(n-1)(n-4)}{2}$ paths. Thus $\theta = \theta_a = \frac{(n-1)(n-2)}{2}$ \square

Theorem 3.7. If $G = K_{2n} - I, \theta_a(G) = 2n(n-1)$ and $\theta(G) = \frac{n(n-1)}{2}, n > 2$, where I is the one factor of K_{2n}

Proof. In $K_{2n} - I$, there will be n pair of vertices which are non adjacent. For a vertex $v, d(v) = n - 1$. Note that every vertex of G are transit identical. There will be $n - 1$ number of $msp(v)$ of length 2. Hence $\theta_a(G) = 2n(n-1)$. Of the n pair of non adjacent vertices taking 2 pair at a time we get a chordless cycle. Hence $\theta(G) = \frac{n(n-1)}{2}$. \square

Theorem 3.8. Let G be a unicyclic graph, with cycle C_r . If the number of vertex of C_r with $d(v) > 2$ is one, then

1. $\theta(G) = C(p, 2) + 2p + 1$
2. $\theta_a(G) = \frac{1}{2}(p^2 + 3p + 2r - 4)$, where p is the number of pendant vertices of G .

Proof. 1. When forming τ_{min} we first include C_r . Corresponding to every pendant vertex, there will be 2 majorized shortest paths connecting it to vertices of the cycle C_r . Thus including $2p$ paths to τ . Again there are $C(p, 2)$ majorized shortest path connecting pendant vertices among themselves. Hence $\theta(G) = C(p, 2) + 2p + 1$



2. Here $\tau_{min} = \mathcal{M}_G$. In the previous case if we exclude C_r and include every majorized shortest path of vertices of C_r , which are r in number, we get \mathcal{M}_G . Note that of these r msp, two of them forms a part of msp connecting pendant vertices to vertices of C_r . Hence we get $\theta_a(G) = \frac{1}{2}(p^2 + 3p + 2r - 4)$. \square

 ISSN(P):2319 – 3786
 Malaya Journal of Matematik
 ISSN(O):2321 – 5666

Theorem 3.9. Let G be a unicyclic graph with cycle C_r . Let u and v be two vertices at a distance $\lfloor \frac{r}{2} \rfloor$ to each other with $d(v_1), d(v_2) > 2$. Let T_1 be a tree with p_1 pendant edges and T_2 be a tree with p_2 pendant edges rooted at u and v respectively. Then

$$\theta(G) = \begin{cases} C(p_1 + p_2, 2) + p_1 + p_2 + 1 & , \text{when } r \text{ is odd} \\ 2p_1p_2 + C(p_1, 2) + C(p_2, 2) + 1 & , \text{when } r \text{ is even} \end{cases}$$

Proof. Since G is unicyclic with cycle C_r , $C_r \in \tau_{min}$.

Case 1

Let u_1, u_2 and v_1, v_2 be the vertices of C_r adjacent to u and v respectively. When r is odd, the msp connecting pendant vertices of T_1 to T_2 is unique. Hence they will be p_1p_2 in number. Either of v_1, v_2 (also u_1, u_2) lie on such msp. Without loss of generality let us assume that u_1 and v_1 lie on these msp. There will be p_1 number of msp connecting pendant vertices of T_1 to v_2 and p_2 number of msp connecting pendant vertices of T_2 to u_2 . Hence we get $\theta(G) = C(p_1 + p_2, 2) + p_1 + p_2 + 1$

Case 2

When r is even $\lfloor \frac{r}{2} \rfloor = \frac{r}{2}$. Hence u and v are diametrically opposite vertices of C_r . For every pendant vertex of T_1 there are 2 msp connecting it to a vertex of T_2 . Altogether there are $2 \times p_1 \times p_2$ number of msp. The number of msp connecting pendant vertices of T_1 among themselves is $C(p_1, 2)$ and the case of T_2 is $C(p_2, 2)$. Thus $\theta(G) = 2p_1p_2 + C(p_1, 2) + C(p_2, 2) + 1$. \square

References

- [1] Harary. F; *Graph Theory*, Addison Wesley, 1969.
- [2] Hendrik Timmerman; Todeschini, Roberto; Viviana Consonni; Raimund Mannhold; Hugo Kubinyi (2002). *Handbook of Molecular Descriptors*. Weinheim: Wiley-VCH. ISBN 3-527-29913-0.
- [3] Melnikov. O, Sarvanov.V, Tyshkevich.R, Yemelichev.V and Zverovich.I: *Exercises in Graph Theory: Section 1.2*
- [4] Reshmi KM; and Raji Pilakkat, Transit Index of a Graph and its correlation with MON of octane isomers(Communicated).
- [5] Reshmi KM; and Raji Pilakkat, Transit Index of various Graph Classes(Communicated).
- [6] Schultz. H. P, *Topological Organic Chemistry. 1. Graph Theory and Topological Indices of Alkanes. J. Chem. Inf. Comput. Sci.* 29, 227-228, 1989.
- [7] Wagner.S; Wang.H, *Introduction to chemical graph theory, Boca Raton, FL : CRC Press, Taylor & Francis Group, [2019]*

