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PERIPHERAL GEODESIC INDEX FOR GRAPHS

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Abstract

In this paper, we introduce a new topological index for graphs called peripheral geodesic index. The peripheral geodesic index is the number of geodesics between peripheral vertices. We computer Peripheral Geodesic Index for some standard graphs. Further, we establish formulae for computing the number of graph geodesics in a graph and the peripheral geodesic index using the adjacency matrix.

1. Introduction

For standard terminology and notion in graph theory, we follow the textbook of Harary [4]. The non-standard will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number

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of edges in a shortest path (also called a graph geodesic) connecting them. The diameter of G, denoted by $d(G)$, is the length of the longest graph geodesic in G. For two vertices u and v in G, $g(u, v)$ denotes the number of geodesics whose end vertices are u and v. The number of geodesics in G is denoted by $f(G)$ or simply f, and f_i denotes the number of geodesics of length i in G. Clearly, $f_i = |E|$ and for a graph of diameter d, we have,

$$f(G) = \sum_{i=1}^{d} f_i \tag{1}$$

It is easy to see that

$$\sum_{\{u, v\} \subset V} g(u, v) = f(G) \tag{2}$$

Using (1), we have the following computations:

1. For a cycle C_n on n vertices,

$$f(C_n) = \begin{cases} \frac{n(n-1)}{2}, & \text{if } n \text{ is odd;} \\ \frac{n^2}{2}, & \text{if } n \text{ is even.} \end{cases} \tag{3}$$

2. For a complete graph K_n on n vertices,

$$f(K_n) = \frac{n(n-1)}{2} \tag{4}$$

3. For the complete bipartite graph $K_{m, n}$,

$$f(K_{m, n}) = \frac{1}{2} mn(m + n) \tag{5}$$

4. For a tree T on n vertices,

$$f(T) = \frac{n(n-1)}{2}. \tag{6}$$

The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G. A vertex with maximum eccentricity in G is called a peripheral vertex in G. So, vertices whose eccentricities are equal to diameter G are peripheral vertices of G. The set of all peripheral vertices of G is denoted by $PV(G)$.

The role of topological indices in drug development research is streamlined. A sequence of definitions in the fields of topological indices and drug discovery technologies are introduced. There are many distance based and degree based topological indices defined for graphs. Wiener index (see [8]) and peripheral Wiener index (see [7]) are two interesting topological indices defined based on graph distance. The Wiener index is substantially used in theoretical chemistry for the design of quantitative structure-property relations (mainly with physicochemical properties) and quantitative structure-activity relations including biological activities of the respective chemical compounds. Since benzenoid hydrocarbons are fascinating the huge significance of theoretical chemists, the theory of the Wiener index of the respective molecular graphs have been extensively developed in the last three decades. The (ordinary) Wiener index $W(G)$ of a connected graph G is defined to be the sum of distances between all vertex pairs in G. The peripheral Wiener index $PW(G)$ of G is defined as the sum of the distances between all pairs of peripheral vertices of G.

In this paper, we introduce a new topological index for graphs called Peripheral Geodesic Index: the peripheral geodesic index $Pg(G)$ of a graph G is defined as the number of geodesics between peripheral vertices of G. We compute Peripheral Geodesic Index for some standard graphs. Further we establish formulae for computing the number of graph geodesics in a graph and the peripheral geodesic index using the adjacency matrix.

2. Peripheral Geodesic Index

Definition 2.1. The peripheral geodesic index $Pg(G)$ of a graph G is defined as the number of geodesics between peripheral vertices of G i.e.,

$$Pg(G) = \sum_{\{u,\, v\} \subset PV(G)} g(u,\, v) \tag{7}$$

Observation: If there are k peripheral vertices in a (connected) graph G, then we have $\binom{k}{2}$ pairs of peripheral vertices and there is at least one path between each pair and hence, we have,

$$\binom{k}{2} \leq Pg(G) \leq f(G).$$

Example 2.2. We compute the peripheral geodesic index of hydrogen-depleted molecular graph G of 1-Ethyl-2-methylcyclobutane C_7H_{14}. We label the vertices of G (see Figure 1).

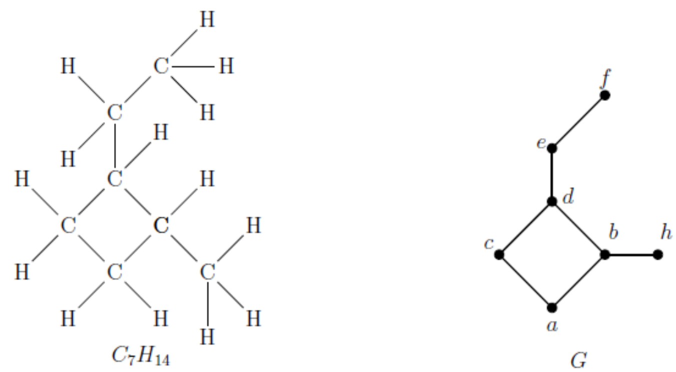

Figure 1. 1-Ethyl-2-methylcyclobutane C_7H_{14} and the corresponding hydrogen-depleted molecular graph G.

Here, $PV(G) = \{a, f, h\}$. We have $g(a, f) = 2$, $g(a, h) = 1$, and $g(f, h) = 1$. The peripheral geodesic index of G is

$$Pg(G) = g(a, f) + g(a, h) + g(f, h)$$
$$= 2 + 1 + 1$$
$$= 4.$$

Proposition 2.3. *If G is a graph with $PV(G) = V(G)$, then $Pg(G) = f(G)$.*

Proof. Obvious. □

Corollary 2.4. 1. *For a cycle C_n on n vertices,*

$$Pg(C_n) = \begin{cases} \dfrac{n(n-1)}{2}, & \text{if } n \text{ is odd;} \\ \dfrac{n^2}{2}, & \text{if } n \text{ is even.} \end{cases}$$

2. *For a complete graph* K_n *on n vertices,* $Pg(K_n) = \dfrac{n(n-1)}{2}$.

3. *For the complete bipartite graph* $K_{m,\, n}$,

$$Pg(K_{m,\, n}) = \frac{1}{2} mn(m+n).$$

Proof. In C_n, K_n and $K_{m,\, n}$, all the vertices peripheral vertices. Hence $PV(C_n) = V(C_n)$, $PV(K_n) = V(K_n)$ and $PV(K_{m,\, n}) = V(K_{m,\, n})$, and the proof follows by the Proposition 2.3 and the equations (3), (4) and (5).

Proposition 2.5. *For a tree T with* $k \geq 2$ *peripheral vertices,*

$$Pg(T) = \frac{k(k-1)}{2}.$$

Proof. Let $PV(T) = \{v_1, v_2, \ldots, v_k\}$. Since there is one and only one path between any two vertices in a tree, it follows that

$$Pg(T) = \sum_{1 \leq i < j \leq k} g(v_i, v_j) = \sum_{1 \leq i < j \leq k} 1 = \binom{k}{2} = \frac{k(k-1)}{2}. \qquad \square$$

Corollary 2.6. 1. *For a path* P_n *on* $n \geq 2$ *vertices,* $Pg(P_n) = 1$.

2. *For a star* $K_{1,\, n}$ *on* $n+1$ *vertices,* $Pg(K_{1,\, n}) = \dfrac{n(n-1)}{2}$.

Proof. There are 2 pendant vertices in P_n and there are n pendant vertices in $K_{1,\, n}$. Hence the proof follows by Proposition 2.5. $\square$

Proposition 2.7. *Let* $Wd(n, m)$ *denotes the windmill graph constructed for* $n \geq 2$ *and* $m \geq 2$ *by joining* m *copies of the complete graph* K_n *at a shared common vertex v. Then by the equation* (7), *we have*

$$Pg(Wd(n, m)) = \frac{m(n-1)(n-2)}{2} + \frac{m(m-1)(n-1)^2}{2}.$$

Hence, for the friendship graph F_k on $2k+1$ vertices,

$$Pg(F_k) = k(2k-1).$$

Proof. Since there are m copies of K_n in $Wd(n, m)$ and their vertices are adjacent to v, it follows that, the diameter of $Wd(n, m)$ is 2 and $PV(Wd(n, m)) = V - v$. Let $H_1, \ldots, H_n$ be the components of $Wd(n, m) - v$. Note that $H_i \cong K_{n-1}, \forall i$ and for any $u, v \in PV(Wd(n, m)), u \neq v$, we have,

$$g(u, v) = 1.$$

Hence from (7) we have

$$\begin{aligned} Pg(Wd(n, m)) &= \sum_{\{u, v\} \subset (Wd(n, m))} g(u, v) \\ &= \sum_{\substack{\{u, v\} \subset V(H_i), \\ \text{for some } i,\, 1 \le i \le m}} 1 + \sum_{\substack{u \in V(H_i),\, v \in V(H_j) \\ i \neq j,\, 1 \le i < j \le m}} 1 \\ &= m\binom{n-1}{2} + \frac{1}{2} m(n-1)(n-1)(m-1) \\ &= \frac{m(n-1)(n-2)}{2} + \frac{m(m-1)(n-1)^2}{2}. \end{aligned}$$

Since the friendship graph F_k on $2k+1$ vertices is nothing but $Wd(3, k)$, it follows that

$$\begin{aligned} Pg(F_k) &= \frac{k(3-1)(3-2)}{2} + \frac{k(k-1)(3-1)^2}{2} \\ &= k(2k-1). \end{aligned}$$

□

Proposition 2.8. *For the wheel graph W_n on $n \geq 4$ vertices,*

$$Pg(W_n) = \frac{n(n-1)}{2}.$$

Proof. We recall that,

$$d(W_n) = \begin{cases} 1, & \text{if } n = 4; \\ 2, & \text{if } n \geq 5, \end{cases}$$

and in W_n, $n \geq 5$, there are $n-1$ peripheral vertices and one central vertex. We have $W_4 = K_4$, and so $Pg(W_4) = \frac{1}{2} 4(4-1) = 6$ (from Corollary 2.4).

In W_5, there are 4 peripheral vertices. Let v be a peripheral vertex in W_5. There are exactly 2 peripheral vertices adjacent to v and there is a vertex at distance 2 with 3 geodesics between this vertex and v. Therefore there are $1+1+3=5$ geodesics from v to other peripheral vertices. Since there are 4 peripheral vertices, $Pg(W_5) = \frac{1}{2} \cdot 4 \cdot 5 = 10$.

In W_6, there are 5 peripheral vertices. Let v be a peripheral vertex in W_6. There are exactly 2 peripheral vertices adjacent to v. There are 2 vertices at distance 2 and there are 2 geodesics between v and each of them. Therefore there are $1+1+2+2=6$ geodesics from v to other peripheral vertices. Since there are 5 peripheral vertices, $Pg(W_6) = \frac{1}{2} \cdot 5 \cdot 6 = 15$.

In W_n, $n \geq 7$, there are $n-1$ peripheral vertices. Let v be a peripheral vertex. There are exactly 2 peripheral vertices adjacent to v. There are exactly 2 vertices at distance 2, and there are 2 geodesics between v and each of them. There are exactly $n-1-5=n-6$ peripheral vertices are at distance 2, and there is exactly one geodesic between v and each of them. Therefore there are $1 \cdot 2 + 2 \cdot 2 + 1 \cdot (n-6) = n$ geodesics from v to other peripheral vertices. Since there are $n-1$ peripheral vertices, $Pg(W_n) = \frac{1}{2}(n-1)(n)$. Thus, $Pg(W_n) = \frac{n(n-1)}{2}$, for $n \geq 4$.

Proposition 2.9. *For the $m \times n$ grid graph $P_m \square P_n$ (the graph Cartesian product of path graphs on m and n vertices),*

$$Pg(P_m \square P_n) = 2\left[2 + \frac{(m+n-2)!}{(m-1)!\,(n-1)!}\right].$$

Hence, for the ladder graph $P_m \square P_2$,

$$Pg(P_m \square P_2) = 2n + 4.$$

Proof. In the grid graph $P_m \square P_n$, there are 4 peripheral vertices situated at the four corners of the grid. Let v be peripheral vertex. There is exactly one peripheral vertex at the distance $(m-1)$ from v and there is exactly one geodesic between this vertex and v. There is exactly one peripheral vertex at the distance $(n-1)$ from v and there is exactly one geodesic between this vertex and v. There is exactly one peripheral vertex (at opposite corner of v) at the distance $(m+n-2)$ from v and it is esy to see that there are exactly $\binom{m+n-2}{m-1}$ geodesics between this vertex and v. Therefore there are $1 + 1 + \binom{m+n-2}{m-1} = 2 + \frac{(m+n-2)!}{(m-1)!(n-1)!}$ geodesics from v to other peripheral vertices. Since there are 4 peripheral vertices,

$$\begin{aligned} Pg(P_n \square P_2) &= \frac{1}{2} \cdot 4\left[2 + \frac{(m+n-2)!}{(m-1)!(n-1)!}\right] \\ &= 2\left[2 + \frac{(m+n-2)!}{(m-1)!(n-1)!}\right] \end{aligned} \tag{8}$$

From (8), for the ladder graph $P_m \square P_2$, it follows that,

$$\begin{aligned} Pg(P_n \square P_2) &= 2\left[2 + \frac{n!}{(n-1)!}\right] \\ &= 2n + 4. \end{aligned}$$ □

2.1 Computation of number of geodesics in a graph and peripheral geodesic index using adjacency matrix

Let G be a graph of diameter d with n vertices $v_1, \ldots, v_n$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of the graph G, where

$$a_{ij}^{(1)} = \begin{cases} 1, & \text{if } v_i \sim v_j; \\ 0, & \text{otherwise.} \end{cases}$$

We consider the following powers of $A : A^2, \ldots, A^d$, where d is the diameter of G. We denote the (i, j)-th element of $A^t(2 \leq t \leq d)$, by $a_{ij}^{(t)}$, where

$$a_{ij}^{(t)} = \sum_{k=1}^{n} a_{ik}^{(t-1)} a_{kj}^{(1)}.$$

We know that $a_{ij}^{(t)}$ is the number distinct edge sequences between v_i and v_j of length t. Let g_{ij} be the first non-zero entry in the sequence $a_{ij}^{(1)}, a_{ij}^{(2)}, \ldots, a_{ij}^{(d)}$. Clearly, g_{ij} is the number of geodesics between v_i and v_j, i.e., $g(v_i, v_j) = g_{ij}$. Therefore the number of geodesics in G is given by

$$f(G) = \sum_{1 \leq i < j \leq n} g_{ij} \tag{9}$$

Let us define $\psi_{ij}^{(t)}, (1 \leq t \leq d - 1)$ as follows:

$$\psi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \ldots = a_{ij}^{(t)} = 0; \\ 0, & \text{otherwise} \end{cases} \tag{10}$$

Then the number of geodesics of length $l \, (1 \leq l \leq d)$ in G, is given by

$$f_l = \sum_{1 \leq i < j \leq n} \psi_{ij}^{(l-1)} a_{ij}^{(l)} \tag{11}$$

Since $f(G) = f_1 + f_2 + \ldots + f_d$ and $f_1 = |E(G)|$, using (11), we have

$$f(G) = \sum_{l=1}^{d} \sum_{1 \leq i < j \leq n} \psi_{ij}^{(l-1)} a_{ij}^{(l)} = |E(G)| + \sum_{l=2}^{d} \sum_{1 \leq i < j \leq n} \psi_{ij}^{(l-1)} a_{ij}^{(l)} \tag{12}$$

Let us define $\phi_{ij}^{(t)}, (1 \leq t \leq d)$ as follows:

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \ldots = a_{ij}^{(t)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise} \end{cases} \tag{13}$$

Then

$$g_{ij} = a_{ij}^{(1)} \cdot \phi_{ij}^{(1)} + a_{ij}^{(2)} \cdot \phi_{ij}^{(2)} + \ldots + a_{ij}^{(d)} \cdot \phi_{ij}^{(d)} = \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{14}$$

and using this in (9), we write

$$f(G) = \sum_{1 \le i < j \le n} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{15}$$

Suppose that G has k peripheral vertices. Without loss of generality we may assume that $v_1, \ldots, v_k$ are the peripheral vertices of G. Then,

$$Pg(G) = \sum_{1 \le i < j \le k} g_{ij} \tag{16}$$

Using (14) in (16), we get

$$Pg(G) = \sum_{1 \le i < j \le k} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{17}$$

Thus we have.

Theorem 2.10. *Let G be a (connected) graph of diameter d with $n \ge 2$ vertices $v_1, \ldots, v_n$ and k peripheral vertices $v_1, \ldots, v_k$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of G and (i, j)-th element of $A^t (2 \le t \le d)$, is denoted by $a_{ij}^{(t)}$.* Then

$$f(G) = \sum_{l=1}^{d} \sum_{1 \le i < j \le n} \psi_{ij}^{(l-1)} a_{ij}^{(l)} = |E(G)| + \sum_{l=2}^{d} \sum_{1 \le i < j \le n} \psi_{ij}^{(l-1)} a_{ij}^{(l)},$$

$$f(G) = \sum_{1 \le i < j \le n} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)}$$

and

$$Pg(G) = \sum_{1 \le i < j \le k} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)}$$

where $\psi_{ij}^{(t)}$, $(1 \leq t \leq d-1)$ is given by

$$\psi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \dots = a_{ij}^{(t)} = 0; \\ 0, & \text{otherwise} \end{cases}$$

and $\phi_{ij}^{(t)}$, $(1 \leq t \leq d)$ is given by

$$\psi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \dots = a_{ij}^{(t)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise} \end{cases}$$

Conclusion

All graphs considered in this manuscript are simple and connected. We have introduced a new topological index for graphs called peripheral geodesic index. Also, we computed peripheral geodesic index $Pg(G)$ for some standard graphs. Further, we have established formulae for computing the number of graph geodesics in a graph and the peripheral geodesic index using the adjacency matrix. A large number of molecular-graph-based structure descriptors (topological indices) based on degrees of vertices and distance between vertices. But in this paper, we have defined the new topological index for graphs without using the degrees of vertices and distance between vertices. This index can be used to determine properties of various classes of graphs and results in this direction will be reported in a subsequent paper.

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