

A STUDY ON RATIONAL METRIC ENERGY OF A GRAPH

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Abstract

The concept of energy of a graph plays an important role in different fields of science and engineering. We consider simple, finite and undirected graphs throughout this paper. The energy, $E(G)$ of a simple graph G is defined to be the sum of the absolute values of the eigen values of G . For any two vertices $u, v \in V(G)$, $d(u/v)$ the rational distance from u to v is given by $d(u/v) = \frac{\sum_{u_i \in N[u]} d(u_i, v)}{\deg(u)+1}$. The rational distance matrix $M_R(G) = [a_{ij}]$ of a graph G is a square matrix of order n , where $a_{ij} = 0$ if $i = j$ and $a_{ij} = d(v_i/v_j)$ if $i \neq j$. If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigen values of the rational distance matrix, then $\sum_{i=1}^n |\lambda_i|$ is called the Rational metric energy of the graph G and is denoted by $E_{MR}(G)$. In this paper we obtain the rational metric energy of some family of graphs and compare the results with the usual energies of graphs.

Key Words : *Rational distance, Rational metric, Rational distance matrix.*

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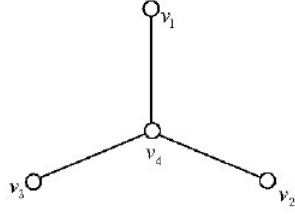
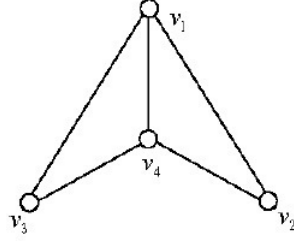
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1. Introduction

In this paper we define distance from a vertex to another vertex in a new way. We would like to give importance to a vertex by its proximity along with its related factors, so define rational distance.

The rational distance takes the neighborhood vertices into account along with the vertex. This will have a better reflection in the case of biological or sociological applications. A vertex in a real sense represents a situation. Therefore all the factors influencing it can be considered. With the help of rational distance, we can define many of the graph invariants in a new way. We refer the definitions and results in [1, 2, 3, 4, 5, 6, 7] by various authors.

1. A Graph $G = (V, E)$ is an ordered pair consisting of a nonempty set $V = V(G)$ of elements called vertices and $E = E(G)$ of unordered pairs of vertices called edges.
2. A Wheel $W_{1,n}$ is a graph defined for any integer $n \geq 3$, which is a graph of order $n + 1$ with one vertex of degree n which is a central vertex and all remaining vertices are of degree 3, called as rim vertices.
3. Suppose $V(G) = \{v_1, v_2, \dots, v_n\}$. The adjacency matrix $A(G)$ of the graph G is a square matrix of order n , such that $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$ otherwise.
4. The eigen values of a graph G are defined as the eigen values of its adjacency matrix $A = A(G)$. That is the roots of the characteristic polynomial $\det(\lambda I_n - A)$ of the adjacency matrix.
5. If $\lambda_1, \lambda_2, \dots, \lambda_n$ are eigen values of a graph G , then the energy of G is given by
$$E(G) = \sum_{i=1}^n |\lambda_i|.$$
6. For any two vertices $u, v \in V(G)$, $d(u, v)$ denote the length of the shortest path between u and v called the distance between u and v .
7. The distance matrix $D(G)$ of a graph G is a square matrix of order n where $a_{ij} = d(v_i, v_j)$.

Figure 1: The Graph G_1 .Figure 2: The Graph G_2 .

8. Wiener index of a graph is defined as the sum of the lengths of the shortest paths between all vertices. Suppose $D = (a_{ij})$ is the distance matrix of a graph G , then Wiener index of G is given by $\frac{1}{2} \sum a_{ij}$.
9. Suppose $\lambda_1, \lambda_2, \dots, \lambda_n$ are eigen values of distance matrix $D(G)$, then the distance energy $E_D(G)$ of a graph G is given by $E_D(G) = \sum_{i=1}^n |\lambda_i|$.

Definition 1.1 : For any two vertices $u, v \in V(G)$, $d(u/v)$ gives the rational distance from u to v given by, $d(u/v) = \frac{\sum_{u_i \in N[u]} d(u_i, v)}{\deg(u) + 1}$.

The following example illustrates the main advantage of rational metric in a graph. In graph G_1 , the country v_1 is in alliance with only country v_4 and country v_4 is in alliance with countries v_2 and v_3 . Then rational distance from v_1 to v_4 is $\frac{5}{4}$. In graph G_2 , country v_1 is in alliance with v_4 and also with countries v_2 and v_3 which are in alliance with v_4 . Now rational distance from v_1 to v_4 is $\frac{3}{4}$, which means distance from v_1 to v_4 has been reduced. Therefore relationship between v_1 and v_4 is improved. We can use this concept for analysing personal relationship among people or to analyse chemical bonding between atoms.

For the graph in Figure 1, $D(G_1) = \begin{bmatrix} 0 & 2 & 2 & 1 \\ 2 & 0 & 2 & 1 \\ 2 & 2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$.

Eigen values of $D(G_1)$ are $-2, -2, -0.6457513, 4.6457513$.

Distance energy of G , $E_D(G_1) = 2 + 2 + 0.6457513 + 4.6457513 = 9.291502$.

2. Rational Metric Energy

Theorem 2.1: For any two vertices u and v in a graph G ,

$$d(u, v) - \frac{k}{k+1} \leq d(u/v) \leq d(u, v) + \frac{k}{k+1}.$$

Proof : For any two vertices u and v , $d(u/v) = \frac{\sum_{u_i \in N[u]} d(v, u_i)}{\deg(u)+1}$. If $w \in N(u)$, then $d(v, w) = d(v, u)$ or $d(v, w) = d(u, v) \pm 1$. Suppose all the vertices in $N(u)$ are at distance $d(u, v) = 1$ from v then

$$\begin{aligned} d(u/v) &= \frac{d(u, v) + k[d(u, v) + 1]}{k+1} \\ &= (u, v) + \frac{k}{k+1}. \end{aligned}$$

Suppose all the vertices in $N(u)$ are at distance $d(v, u) - 1$ from v , then

$$\begin{aligned} d(u/v) &= \frac{d(u, v) + k[d(u, v) - 1]}{k+1} \\ &= (u, v) - \frac{k}{k+1}. \end{aligned}$$

□

Definition 2.2 : The rational distance matrix $M_R(G) = [a_{ij}]$ of a graph G is a square matrix of order n , where $a_{ij} = 0$ if $i = j$ and $a_{ij} = d(v_i/v_j)$ if $i \neq j$.

Definition 2.3 : If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigen values of the rational distance matrix, then $\sum_{i=1}^n |\lambda_i|$ is called the Rational metric energy of the graph G .

For the graph in Figure 1,

$$M_R(G_1) = \begin{bmatrix} 0 & 1.5 & 1.5 & 0.5 \\ 1.5 & 0 & 1.5 & 0.5 \\ 1.5 & 1.5 & 0 & 0.5 \\ 1.24 & 1.24 & 1.24 & 0 \end{bmatrix}$$

Eigen values of $M_R(G_1)$ are 3.5310096, -1.5 , -0.5310096 , -1.5 and the Rational Metric energy of G , $E_{MR}(G) = 3.5310096 + 1.5 + 0.5310096 + 1.5 = 7.0620192$.

Definition 2.4 : For two vertices $u, v \in V(G)$, symmetric rational distance between u and v is given by $\frac{d(u/v) + d(v/u)}{2}$.

In the G_1 of Figure 1, the symmetric rational distance between v_1 and v_4 is $\frac{0.5+1.24}{2} = 0.87$.

Now we compare three types of energies discussed above for a wheel W_1, n for different values of n .

The graph	Graph Energy	distance Energy	Rational distance Energy
$W_{1,3}$	6	6	4.5
$W_{1,4}$	6.472136	9.6568542	8
$W_{1,5}$	9.3711129	13.4882614	11.5192024
$W_{1,6}$	11.291503	17.380832	15.0388694

2.1 Rational Diameter of a Graph

Definition 2.5 : Rational diameter of a graph is given by largest entry in the rational distance matrix, denoted by $diam_R(G)$.

Theorem 2.6 : For a connected graph G , Rational diameter of G cannot exceed the diameter of the graph.

Proof : Let $diam(G) = d(u, v)$ for some $u, v \in G$ and let $diam_R(G) = d(u_1/v_1)$ for some $u_1, v_1 \in G$. If $d(u, v) = d(u_1, v_1)$, then u_1 is a farthest vertex from v_1 in G and hence $d(u_1/v_1) \leq d(u_1, v_1)$. Assume that $d(u, v) > d(u_1, v_1)$. Then,

$$d(u_1, v_1) \leq d(u, v) - 1. \quad (1)$$

But, $d(u_1/v_1) \leq d(u_1, v_1) + \frac{k}{k+1}$, where k is degree of the vertex v_1 . Which implies $d(u_1, v_1) \geq d(u_1/v_1) - \frac{k}{k+1}$. By 1,

$$d(u_1/v_1) - \frac{k}{k+1} \leq d(u_1, v_1) \leq d(u, v) - 1$$

$$\Rightarrow d(u_1/v_1) + 1 - \frac{k}{k+1} \leq d(u, v).$$

Since $1 - \frac{k}{k+1}$ is a positive fraction, $d(u_1/v_1) < d(u, v)$. Hence $d(u/v) < d(u, v)$. \square

Remark 2.7 : Suppose $diam(G) = d(u, v)$, then $diam_R(G)$ need not be equal to $d(u/v)$. Consider the graph $G = K_{1,6}$, where u, v be any two vertices of degree one and w be the central vertex. Then $diam(G) = d(u, v) = 2$ and $diam_R(G) = d(u/w) = 1.57$.

Now we determine rational diameter of some simple classes of graphs.

Theorem 2.8 : For a path P_n $diam_R(G) = \frac{2n-1}{2}$.

Proof : Consider a path P_n with vertices v_1, v_2, \dots, v_n , where v_i is adjacent to v_{i+1} for $1 \leq i \leq n-1$. Then $\text{diam}(G) = d(v_1, v_n)$. Therefore,

$$\begin{aligned}
 \text{diam}_R &= d(v_1 v_n) \\
 &= \frac{\sum_{u \in N[v_1]} d(v_1, u)}{\deg(v_1) + 1} \\
 &= \frac{d(v_1, v_n) + d(v_2, v_n)}{2} \\
 &= \frac{n + n - 1}{2} \\
 &= \frac{2n - 1}{2}.
 \end{aligned}$$

□

Theorem 2.9 : For a cycle C_n , $\text{diam}_R(C_n) = \frac{n}{2} - \frac{2}{3}$ if n is even and $\text{diam}_R(C_n) = \frac{n-1}{2} - \frac{1}{3}$ if n is odd.

Proof : Consider a cycle C_n with vertices v_1, v_2, \dots, v_n , where v_i is adjacent to v_{i+1} for $1 \leq i \leq n-1$ and v_n is adjacent to v_1 .

Case 1 : n is even.

Then $\text{diam}(C_n) = d(v_1, v_{\frac{n}{2}+1}) = n/2$.

$$\begin{aligned}
 \text{diam}_R(C_n) &= d(v_1, v_{\frac{n}{2}+1}) \\
 &= \frac{\sum_{u \in N[v_1]} d(v_1, u)}{\deg(v_1) + 1} \\
 &= \frac{d(v_1, v_{\frac{n}{2}+1}) + d(v_{\frac{n}{2}+1}, v_2) + d(v_{\frac{n}{2}+1}, v_n)}{3} \\
 &= \frac{\frac{n}{2} + \frac{n}{2} - 1 + \frac{n}{2} - 1}{3} \\
 &= \frac{n}{2} - \frac{2}{3}.
 \end{aligned}$$

Case 2 : n is odd.

Then $diam(C_n) = d(v_1, v_{\frac{n-1}{2}+1}) = \frac{n-1}{2}$.

$$\begin{aligned}
 diam_R(C_n) &= d(v_1/v_{\frac{n-1}{2}+1}) \\
 &= \frac{\sum_{u \in N[v_1]} d(v_{\frac{n-1}{2}+1}, u)}{deg v_1 + 1} \\
 &= \frac{d(v_1, v_{\frac{n-1}{2}+1}) + d(v_{\frac{n-1}{2}+1}, v_2) + d(v_{\frac{n-1}{2}+1}, v_n)}{3} \\
 &= \frac{\frac{n-1}{2} + \frac{n-1}{2} - 1 + \frac{n-1}{2} - 1}{3} \\
 &= \frac{n-1}{2} - \frac{1}{3}.
 \end{aligned}$$

2.2 Rational Wiener Index

The Wiener index of a graph is dependent on distances between vertices. Therefore with the introduction of rational distance, we can define an alternative to Wiener index. This rational Wiener index, which will be less than wiener index and can play significant role in analyzing bonds between atoms in a molecule, there by can give reasons for certain abnormal properties of some chemicals.

Definition 2.10 : Suppose $D_R(G) = (R_{ij})$ is the Rational distance matrix of a graph G , then the Rational Wiener Index of G is given by $\frac{1}{2} \sum R_{ij}$.

Theorem 2.11 : For an odd cycle C_n , Rational wiener index is given by,

$$W_R(C_n) = \frac{n}{2} \left[\frac{(n-1)(n+1)}{4} - \frac{2}{3} \right].$$

Proof : Consider a cycle C_n with vertices v_1, v_2, \dots, v_n , where v_i is adjacent to v_{i+1} for $1 \leq i \leq n-1$ and v_n is adjacent to v_1 .

Then $n = 2k + 1$ for some integer k . Note that;

$$W_R(C_n) = \frac{1}{2} \sum_{u_i \in V(C_n)} d(u/v).$$

In C_n , for any $l = 1, 2, \dots, n$;

$$d(v_i/v_j) = \begin{cases} 0, & i = j \\ 1, & d(v_i, v_j) = 1 \\ 2, & d(v_i, v_j) = 2 \\ \vdots & \\ k-1, & d(v_i, v_j) = k-1 \\ k - \frac{1}{3}, & d(v_i, v_j) = k \end{cases}$$

For a fixed l , $1 \leq l \leq n$, we have $d(v_l/v_i) = d(v_l/v_j)$ if $d(v_l, v_i) = d(v_l, v_j)$. Therefore $\sum d(v_i/v_j) = 2n[0+1+\dots+(k-1)+k-\frac{1}{3}]$ and $W_R(C_n) \frac{1}{2} \sum d(v_i/v_j) = n \left[\frac{k(k+1)}{2} - \frac{1}{3} \right] = \frac{n}{2} \left[\frac{(n-1)(n+1)}{4} - \frac{2}{3} \right]$.

Theorem 2.12 : For an even cycle C_n Rational wiener index $W_R(C_n) = \frac{n}{2} \left[\frac{n^2}{4} - \frac{2}{3} \right]$.

Proof : Consider a cycle C_n with vertices v_1, v_2, \dots, v_n , where v_i is adjacent to v_{i+1} for $1 \leq i \leq n-1$ and v_n is adjacent to v_1 . Then $n = 2k$ for some integer k . Note that $W_R(C_n) = \frac{1}{2} \sum_{u,v \in V(C_n)} d(u/v)$. In C_n , for any $1, 2, \dots, n$.

$$d(v_i/v_j) = \begin{cases} 0, & i = j \\ 1, & d(v_i, v_j) = 1 \\ 2, & d(v_i, v_j) = 2 \\ \vdots & \\ k-1, & d(v_i, v_j) = k-1 \\ k-\frac{2}{3}, & d(v_i, v_j) = k \end{cases}$$

For a fixed l , $1 \leq l \leq n$, we have $d(v_l/v_i) = d(v_l/v_j)$ if $d(v_l, v_i) = d(v_l, v_j)$. Also we note that $d(v_i/v_j) = k - \frac{2}{3}$ if $d(v_i, v_j) = \frac{n}{2}$. Therefore, $\sum d(v_i/v_j) = n[2(0+1+\dots+(k-1))+k-\frac{2}{3}]$ and $W_R(C_n) = \frac{1}{2} \sum d(v_i/v_j) = \frac{n}{2} \left[\frac{2k(k-1)}{2} - \frac{2}{3} \right] = \frac{n}{2} \left[\frac{n^2}{4} - \frac{2}{3} \right]$. \square

Now we compare two types of Wiener index discussed above for a wheel $W_{1,n}$ for different values of n .

Wheel	Wiener Index	Rational Wiener Index
$W_{1,3}$	6	6
$W_{1,4}$	12	10.2
$W_{1,5}$	20	17.2916
$W_{1,6}$	30	28.285814

3. Conclusion

In this paper we have defined new versions of graph invariants, which will be more suitable in practical situations. This can be extended to all the other graph invariants and applications.

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