Electronic Journal of Graph Theory and Applications **3** (2) (2015), 228–236

Electronic Journal of
Graph Theory and Applications

Reciprocal complementary distance spectra and reciprocal complementary distance energy of line graphs of regular graphs

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Abstract

The reciprocal complementary distance (RCD) matrix of a graph G is defined as $RCD(G) = [rc_{ij}]$ where $rc_{ij} = \frac{1}{1+D-d_{ij}}$ if $i \neq j$ and $rc_{ij} = 0$, otherwise, where D is the diameter of G and d_{ij} is the distance between the vertices v_i and v_j in G. The RCD-energy of G is defined as the sum of the absolute values of the eigenvalues of $RCD(G)$. Two graphs are said to be RCD-equienergetic if they have same RCD-energy. In this paper we show that the line graph of certain regular graphs has exactly one positive RCD-eigenvalue. Further we show that RCD-energy of line graph of these regular graphs is solely depends on the order and regularity of G. This results enables to construct pairs of RCD-equienergetic graphs of same order and having different RCD-eigenvalues.

Keywords: Reciprocal complementary distance eigenvalues, adjacency eigenvalues, line graphs, reciprocal complementary distance energy
Mathematics Subject Classification : 05C50, 05C12
DOI: 10.5614/ejgta.2015.3.2.10

1. Introduction

Molecular matrices, encoding in various ways the topological infromation, are an important source of structural descriptors for quantitative structure property relationships (QSPR) and quantitative structure activity relationships (QSAR) models [6]. A large number of molecular matrices

Received: 01 June 2015, Revised: 08 September 2015, Accepted: 13 October 2015.

were defined in the chemical literature. One of these is reciprocal complementary distance (RCD) matrix.

Let G be a simple, undirected, connected graph with n vertices and m edges. Let the vertices of G be labeled as $v_1, v_2, \ldots, v_n$. The *adjacency matrix* of a graph G is the square matrix $A = A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if v_i is adjacent to v_j and $a_{ij} = 0$, otherwise. The eigenvalues of the adjacency matrix $A(G)$ are the *adjacency eigenvalues* of G , and these will be labeled as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and their collection is called as a *adjacency spectra* of G [3].

The *distance* between the vertices v_i and v_j, denoted by d_{ij} , is the length of the shortest path between them. The *diameter* of a graph G, denoted by $diam(G)$, is the maximum distance between any pair of vertices of G. A graph G is said to be r*-regular graph* if all of its vertices have same degree equal to r.

The *reciprocal complementary distance* between the vertices v_i and v_j, denoted by rc_{ij} is defined as $rc_{ij} = \frac{1}{1+D-d_{ij}}$, where D is the diameter of G and d_{ij} is the distance between v_i and v_j in G.

The *reciprocal complementary distance matrix* [6, 7] of a graph G is an $n \times n$ real symmetric matrix $RCD(G) = [rc_{ij}]$, where

$$rc_{ij} = \begin{cases} \frac{1}{1+D-d_{ij}}, & \text{if} \quad i \neq j \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues of $RCD(G)$ labeled as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are said to be the ***RCD-eigenvalues*** of G and their collection is called ***RCD-spectra*** of G. Two non-isomorphic graphs are said to be ***RCD-cospectral*** if they have same RCD-spectra.

The *reciprocal complementary distance energy* (RCD*-energy*) of a graph G is defined as

$$RCDE(G) = \sum_{i=1}^{n} |\mu_i| \,. \tag{1}$$

The Eq. (1) is defined in full analogy with the *ordinary graph energy* $E(G)$, defined as [4]

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \,. \tag{2}$$

Two graphs G_1 and G_2 are said to be *equienergetic* if $E(G_1) = E(G_2)$ [1, 2, 8, 11, 12, 16]. For more details on $E(G)$ one can refer [8].

Two connected graphs G_1 and G_2 are said to be *reciprocal complementary distance equienergetic* or ***RCD-equienergetic*** if $RCDE(G_1) = RCDE(G_2)$. Of course, RCD-cospectral graphs are RCD-equienergetic. In this paper we obtain the RCD-eigenvalues and RCD-energy of line graphs of certain regular graphs. Further we show that the RCD-energy of line graphs of certain regular graphs is solely depends on the order and regularity of a graph. Thus infinitely many pairs of RCD-equienergetic graphs can be constructed such that they have equal number of vertices, equal number of edges and are non RCD-cospectral.

We need following results.

Theorem 1.1. [3] *If G is an r-regular graph, then its maximum adjacency eigenvalue is equal to r.*

Theorem 1.2. [13] *Let G be an r-regular graph of order n. If $r, \lambda_2, \ldots, \lambda_n$ are the adjacency eigenvalues of G, then the adjacency eigenvalues of $\overline{G}$, the complement of G, are $n-r-1$ and $-\lambda_i - 1$, $i = 2, 3, \ldots, n$.*

The *line graph* of G, denoted by $L(G)$ is the graph whose vertices corresponds to the edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G [5]. If G is a regular graph of order n and of degree r then the line graph $L(G)$ is a regular graph of order $nr/2$ and of degree $2r-2$.

Theorem 1.3. [14] *If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the adjacency eigenvalues of a regular graph G of order n and of degree r, then the adjacency eigenvalues of $L(G)$ are*

$$\lambda_i + r - 2, \qquad i = 1, 2, \ldots, n, \qquad \textit{and}$$

$$-2, \qquad n(r-2)/2 \ \textit{times}.$$

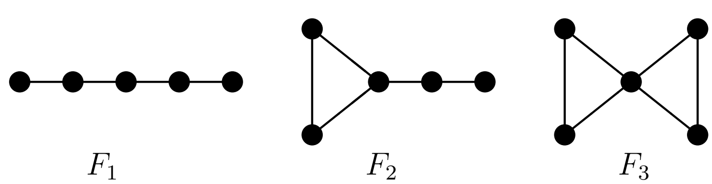

Figure 1: The forbidden induced subgraphs

Theorem 1.4. [9, 10] *For a connected graph G, $diam(L(G)) \leq 2$ if and only if none of the three graphs F_1, F_2 and F_3 of Fig. 1 is an induced subgraph of G.*

Lemma 1.1. [15] *If for any two adjacent vertices u and v of a graph G, there exists a third vertex w which is not adjacent to any of u and v, then*
(i) $\overline{G}$ is connected and
(ii) $diam\left(\overline{G}\right) \leq 2$.

2. RCD-eigenvalues

Theorem 2.1. *Let G be an r-regular graph on n vertices and $diam(G) = 2$. If $r, \lambda_2, \ldots, \lambda_n$ are the adjacency eigenvalues of G, then its RCD-eigenvalues are $n-1-\frac{r}{2}$ and $-1-\frac{\lambda_i}{2}$, $i = 2, 3, \ldots, n$.*

Proof. Since G is an r-regular graph, $\mathbf{1} = [1, 1, \ldots, 1]'$ is an eigenvector of $A = A(G)$ corresponding to the eigenvalue r. Set $\mathbf{z} = \frac{1}{\sqrt{n}}\mathbf{1}$ and let P be an orthogonal matrix with its first column equal to $\mathbf{z}$ such that $P'AP = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Since $diam(G) = 2$, $RCD(G)$ can be written as $RCD(G) = J - I - (1/2)A$, where J is the matrix whose all entries are equal to 1 and I is an identity matrix. It follows that

$$\begin{aligned} P'(RCD)P &= P'\left(J - I - \tfrac{1}{2}A\right)P \\ &= P'JP - I - \tfrac{1}{2}P'AP \\ &= \text{diag}\left(n - 1 - \tfrac{r}{2}, -1 - \tfrac{\lambda_2}{2}, \ldots, -1 - \tfrac{\lambda_n}{2}\right), \end{aligned}$$

where we have used the fact that any column of P other than the first column is orthogonal to the first column. Hence the eigenvalues of $RCD(G)$ are $n - 1 - (r/2)$ and $-1 - (\lambda_i/2)$, $i = 2, 3, \ldots, n$. $\square$

Theorem 2.2. *If G is an r-regular, connected graph of order $n \geq 4$ and if none of the three graphs F_1, F_2 and F_3 of Fig. 1 is an induced subgraph of G, then $L(G)$ has exactly one positive RCD-eigenvalue, equal to $r(n-2)/2$.*

Proof. Let $r, \lambda_2, \lambda_3, \ldots, \lambda_n$ be the adjacency eigenvalues of a regular graph G. Then from Theorem 1.3, the adjacency eigenvalues of $L(G)$ are

$$\left.\begin{array}{rll} \lambda_i + r - 2, & i = 1, 2, \ldots, n, & \text{and} \\ -2, & n(r-2)/2 \ \text{times.} & \end{array}\right\} \tag{3}$$

The graph G is regular of degree r and has order n. Therefore $L(G)$ is a regular graph on $nr/2$ vertices and of degree $2r - 2$. As none of the three graphs F_1, F_2 and F_3 of Fig. 1 is an induced subgraph of G, from Theorem 1.4, $diam(L(G)) = 2$. Therefore from Theorem 2.1 and Eq. (3), the RCD-eigenvalues of $L(G)$ are

$$\left.\begin{array}{rll} r(n-2)/2, & \text{and} & \\ -(\lambda_i + r)/2, & i = 2, 3, \ldots, n & \text{and} \\ 0, & n(r-2)/2 \ \text{times.} & \end{array}\right\} \tag{4}$$

All adjacency eigenvalues of a regular graph of degree r satisfy the condition $-r \leq \lambda_i \leq r$ [3]. Therefore $\lambda_i + r \geq 0$, $i = 1, 2, \ldots, n$. The theorem follows from Eq. (4). $\square$

3. RCD-energy

Theorem 3.1. *If G is an r-regular, connected graph of order $n \geq 4$ and if none of the three graphs F_1, F_2 and F_3 of Fig. 1 is an induced subgraph of G, then*

$$RCDE(L(G)) = r(n-2).$$

Proof. Bearing in mind Theorem 2.2 and Eq. (4), the RCD-energy of $L(G)$ is computed as:

$$\begin{aligned} RCDE(L(G)) &= \frac{r(n-2)}{2} + \sum_{i=2}^{n} \frac{(\lambda_i + r)}{2} + |0| \times \frac{n(r-2)}{2} \\ &= r(n-2) \qquad \text{since} \quad \sum_{i=2}^{n} \lambda_i = -r. \end{aligned}$$

□

From Theorem 3.1, we see that the RCD-energy of the line graph of a regular graph G, that does not contain F_i, $i = 1, 2, 3$, as an induced subgraph is fully determined by the order n and degree r of G.

Let K_n be the *complete graph* on n vertices, $K_{k,k}$ be the *complete bipartite graph* on $2k$ vertices and $CP(k)$ be the *cocktail party graph* (a regular graph on $n = 2k$ vertices and of degree $2k-2$) [3]. None of the three graphs F_1, F_2 and F_3 of Fig.1 is an induced subgraph of these graphs. Therefore from Theorem 3.1 we have following:

Corollary 3.1. (i) $RCDE(L(K_n)) = n^2 - 3n + 2$, *for* $n \geq 4$.
(ii) $RCDE(L(K_{k,k})) = 2k(k-1)$, *for* $k \geq 2$.
(iii) $RCDE(L(CP(k))) = 4(k-1)^2$, *for* $k \geq 2$.

Theorem 3.2. *Let G be an r-regular graph of order n. Let $L(G)$ be the line graph of G such that for any two adjacent vertices u and v of $L(G)$, there exists a third vertex w in $L(G)$ which is not adjacent to any of u and v.*
(i) *If the smallest adjacency eigenvalue of G is greater than or equal to $3-r$, then*

$$RCDE\left(\overline{L(G)}\right) = 3n(r-2)/2.$$

(ii) *If the second largest adjacency eigenvalue of G is at most $3-r$, then*

$$RCDE\left(\overline{L(G)}\right) = (nr/2) + 2r - 3.$$

Proof. Let the adjacency eigenvalues of G be $r, \lambda_2, \ldots, \lambda_n$. From Theorem 1.3, the adjacency eigenvalues of $L(G)$ are

$$\left.\begin{array}{rll} 2r-2, & \text{and} & \\ \lambda_i + r - 2, & i = 2, 3, \ldots, n, & \text{and} \\ -2, & n(r-2)/2 \text{ times.} & \end{array}\right\} \tag{5}$$

From Theorem 1.2 and the Eq. (5), the adjacency eigenvalues of $\overline{L(G)}$ are

$$\left.\begin{array}{rll} (nr/2)-2r+1, & \text{and} & \\ -\lambda_i - r + 1, & i=2,3,\ldots,n, & \text{and} \\ 1, & n(r-2)/2 \text{ times.} & \end{array}\right\} \tag{6}$$

Since for any two adjacent vertices u and v of $L(G)$ there exists a third vertex w which is not adjacent to any of u and v in $L(G)$, by Lemma 1.1, $diam\left(\overline{L(G)}\right)=2$. Therefore by Theorem 2.1 and Eq. (6), the RCD-eigenvalues of $\overline{L(G)}$ are

$$\left.\begin{array}{rll} (nr/4)+r-(3/2), & \text{and} & \\ \frac{\lambda_i+r-3}{2}, & i=2,3,\ldots,n, & \text{and} \\ (-3/2), & n(r-2)/2 \text{ times.} & \end{array}\right\} \tag{7}$$

Therefore

$$RCDE\left(\overline{L(G)}\right)=\left|\frac{nr}{4}+r-\frac{3}{2}\right|+\sum_{i=2}^{n}\left|\frac{\lambda_i+r-3}{2}\right|+\left|-\frac{3}{2}\right|\frac{n(r-2)}{2}. \tag{8}$$

(i) By assumption, $\lambda_i+r-3\geq 0$, $i=2,3,\ldots n$, then from Eq. (8)

$$\begin{aligned} RCDE\left(\overline{L(G)}\right) &= \frac{nr}{4}+r-\frac{3}{2}+\sum_{i=2}^{n}\left(\frac{\lambda_i+r-3}{2}\right)+\frac{3n(r-2)}{4} \\ &= \frac{nr}{4}+r-\frac{3}{2}+\frac{1}{2}\sum_{i=2}^{n}\lambda_i+(n-1)\left(\frac{r-3}{2}\right)+\frac{3n(r-2)}{4} \\ &= \frac{3n(r-2)}{2} \qquad \text{since} \quad \sum_{i=2}^{n}\lambda_i=-r. \end{aligned}$$

(ii) By assumption, $\lambda_i+r-3<0$, $i=2,3,\ldots n$, then from Eq. (8)

$$\begin{aligned} RCDE\left(\overline{L(G)}\right) &= \frac{nr}{4}+r-\frac{3}{2}-\sum_{i=2}^{n}\left(\frac{\lambda_i+r-3}{2}\right)+\frac{3n(r-2)}{4} \\ &= \frac{nr}{4}+r-\frac{3}{2}-\frac{1}{2}\sum_{i=2}^{n}\lambda_i-(n-1)\left(\frac{r-3}{2}\right)+\frac{3n(r-2)}{4} \\ &= \frac{nr}{2}+2r-3 \qquad \text{since} \quad \sum_{i=2}^{n}\lambda_i=-r. \end{aligned}$$

□

Some of the examples of r-regular graphs whose second largest adjacency eigenvalue is at most $3 - r$ and the diameter of the complement of their line graph is equal to two are a 5-vertex cycle C_5, a 5-vertex complete graph K_5, a 6-vertex cycle C_6 and a complete bipartite graph $K_{3,3}$.

Corollary 3.2. *Let G be a cubic graph of order n. Let $L(G)$ be the line graph of G such that for any two adjacent vertices u and v of $L(G)$, there exists a third vertex w in $L(G)$ which is not adjacent to any of u and v. Then*

$$RCDE\left(\overline{L(G)}\right) = \frac{3n + E(G)}{2}.$$

Proof. Substituting $r = 3$ in Eq. (8) we get

$$\begin{aligned} RCDE\left(\overline{L(G)}\right) &= \left|\frac{3n}{4} + \frac{3}{2}\right| + \sum_{i=2}^{n}\left|\frac{\lambda_i}{2}\right| + \left|-\frac{3}{2}\right|\frac{n}{2} \\ &= \frac{3n}{4} + \frac{3}{2} + \frac{1}{2}(E(G) - 3) + \frac{3n}{4} \\ &= \frac{3n + E(G)}{2}. \end{aligned}$$

□

4. RCD-equienergetic graphs

Lemma 4.1. *Let G_1 and G_2 be regular graphs of the same order and of the same degree. Then following holds:*
(i) *$L(G_1)$ and $L(G_2)$ are of the same order, same degree and have the same number of edges.*
(ii) *$\overline{L(G_1)}$ and $\overline{L(G_2)}$ are of the same order, same degree and have the same number of edges.*

Proof. Statement (i) follows from the fact that the line graph of a regular graph is a regular and that the number of edges of G is equal to the number of vertices of $L(G)$. Statement (ii) follows from the fact that the complement of a regular graph is a regular and that the number of vertices of a graph and its complement is equal. □

Lemma 4.2. *Let G_1 and G_2 be regular, connected graphs of the same order $n \geq 4$ and of the same degree. Let none of the three graphs F_1, F_2 and F_3 of Fig. 1 be an induced subgraph of G_i , $i = 1, 2$. Then $L(G_1)$ and $L(G_2)$ are RCD-cospectral if and only if G_1 and G_2 are cospectral.*

Proof. Follows from Eqs. (3) and (4). □

Lemma 4.3. *Let G_1 and G_2 be regular graphs of the same order and of the same degree. Let for $i = 1, 2$, $L(G_i)$ be the line graph of G_i such that for any two adjacent vertices u_i and v_i of $L(G_i)$, there exists a third vertex w_i in $L(G_i)$ which is not adjacent to any of u_i and v_i. Then $\overline{L(G_1)}$ and $\overline{L(G_2)}$ are RCD-cospectral if and only if G_1 and G_2 are cospectral.*

Proof. Follows from Eqs. (5), (6) and (7). □

Theorem 4.1. *Let G_1 and G_2 be regular, connected, non cospectral graphs of the same order $n \geq 4$ and of the same degree r. Let none of the three graphs F_1, F_2 and F_3 of Fig. 1 be an induced subgraph of G_i, $i = 1, 2$. Then line graphs $L(G_1)$ and $L(G_2)$ form a pair of non RCD-cospectral, RCD-equienergetic graphs of equal order and of equal number of edges.*

Proof. Follows from Lemma 4.1, Lemma 4.2 and Theorem 3.1. □

Theorem 4.2. *Let G_1 and G_2 be regular, non cospectral graphs of the same order and of the same degree r. Let for $i = 1, 2$, $L(G_i)$ be the line graph of G_i such that for any two adjacent vertices u_i and v_i of $L(G_i)$, there exists a third vertex w_i in $L(G_i)$ which is not adjacent to any of u_i and v_i.*
(i) *If the smallest adjacency eigenvalue of G_i, $i = 1, 2$ is greater than or equal to $3 - r$, then $\overline{L(G_1)}$ and $\overline{L(G_2)}$ form a pair of non RCD-cospectral, RCD-equienergetic graphs of equal order and of equal number of edges.*
(ii) *If the second largest adjacency eigenvalue of G_i, $i = 1, 2$ is at most $3 - r$, then $\overline{L(G_1)}$ and $\overline{L(G_2)}$ form a pair of non RCD-cospectral, RCD-equienergetic graphs of equal order and of equal number of edges.*

Proof. Follows from Lemma 4.1, Lemma 4.3 and Theorem 3.2. □

Theorem 4.3. *Let G_1 and G_2 be non cospectral, cubic equienergetic graphs of the same order. Let for $i = 1, 2$, $L(G_i)$ be the line graph of G_i such that for any two adjacent vertices u_i and v_i of $L(G_i)$, there exists a third vertex w_i in $L(G_i)$ which is not adjacent to any of u_i and v_i. Then $\overline{L(G_1)}$ and $\overline{L(G_2)}$ form a pair of non RCD-cospectral, RCD-equienergetic graphs of equal order and of equal number of edges.*

Proof. Follows from Lemma 4.1, Lemma 4.3 and Corollary 3.2. □

Acknowledgement

Authors are thankful to anonymous referee for his/her valuable suggestions. The first author H. S. Ramane is thankful to the University Grants Commission (UGC), Govt. of India for support through research grant under UPE FAR-II grant No. F 14-3/2012 (NS/PE). Another author A. S. Yalnaik is thankful to the University Grants Commission (UGC), Govt. of India for support through Rajiv Gandhi National Fellowship No. F1-17.1/2014-15/RGNF-2014-15-SC-KAR-74909.

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