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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 RCDequienergetic 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 RCDeigenvalues.

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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

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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 $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ 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

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

The eigenvalues of RCD(G) labeled as $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$ 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

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

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

$$E(G) = \sum_{i=1}^{n} |\lambda_i| .$$
⁽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 equiener*getic 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 $r, \lambda_2, ..., \lambda_n$ 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, ..., 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 $\lambda_1, \lambda_2, ..., \lambda_n$ are the adjacency eigenvalues of a regular graph G of order n and of degree r, then the adjacency eigenvalues of L(G) are

 $\lambda_i + r - 2,$ i = 1, 2, ..., n, and -2, n(r-2)/2 times.



Figure 1: The forbidden induced subgraphs

Theorem 1.4. [9, 10] For a connected graph G, $diam(L(G)) \le 2$ 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) $diam(\overline{G}) \leq 2$.

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, $\mathbf{1} = [1, 1, ..., 1]'$ 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 $P'AP = \text{diag}(\lambda_1, \lambda_2, ..., \lambda_n)$. 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

$$P'(RCD)P = P'(J - I - \frac{1}{2}A)P$$

= $P'JP - I - \frac{1}{2}P'AP$
= diag $(n - 1 - \frac{r}{2}, -1 - \frac{\lambda_2}{2}, \dots, -1 - \frac{\lambda_n}{2})$,

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, ..., n.

Theorem 2.2. If G is an r-regular, connected graph of order $n \ge 4$ 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

$$\lambda_i + r - 2, \qquad i = 1, 2, \dots, n, \qquad \text{and} \\ -2, \qquad n(r-2)/2 \text{ times.}$$

$$(3)$$

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

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

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

3. RCD-energy

Theorem 3.1. If G is an r-regular, connected graph of order $n \ge 4$ 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:

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

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 $n \ge 4$. (ii) $RCDE(L(K_{k,k})) = 2k(k-1)$, for $k \ge 2$. (iii) $RCDE(L(CP(k))) = 4(k-1)^2$, for $k \ge 2$.

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

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

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

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

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

Therefore

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

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

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

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

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

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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

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

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 $n \ge 4$ 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 $n \ge 4$ 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 $L(G_1)$ and $L(G_2)$ form a pair of non RCD-cospectral, RCD-equienergetic graphs of equal order and of equal number of edges.

(ii) If the second largest adjacency eigenvalue of G_i , i = 1, 2 is at most 3 - r, then $\overline{L(G_1)}$ 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 4.3 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 $L(G_1)$ 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 4.3 and Corollary 3.2.

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