The energy of integral circulant graphs

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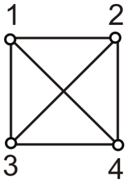
Let G be a simple graph with n vertices and m edges, and let $A = [a_{ij}]$ be the adjacency matrix for G. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A are the eigenvalues of the graph G.

$$A(K_4) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$



$$A \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = 3 \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \qquad A \cdot \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} = -1 \cdot \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

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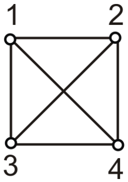

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Definition

The energy of G is introduced by Ivan Gutman in 1978 and defined as the sum of absolute values of its eigenvalues

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

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Motivated by the successes of the theory of graph energy, other energy–like quantities have been proposed, based on the eigenvalues of graph matrices other than the adjacency matrix.

The distance matrix D of a graph G is the square matrix whose (u, v)-entry is the shortest distance between the vertices u and v.

The eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ of the distance matrix are said to be the distance eigenvalues. The distance energy of a graph G is the sum of absolute values of the distance eigenvalues,

$$DE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Distance energy is a useful molecular descriptor in QSPR modeling, as demonstrated by Consonni and Todeschini.

Let $L = D - A$ be the Laplacian matrix of the graph G, and $\mu_1, \mu_2, \ldots, \mu_n$ be its eigenvalues. Then the Laplacian energy of G defined by

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|$$

where n and m denote the number of vertices and edges.

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Two graphs G_1 and G_2 are said to be cospectral if their spectra coincide. In full analogy we speak of pairs of Laplacian cospectral and distance cospectral graphs.

Evidently, cospectral graphs have equal energies.

However, we are interested in finding pairs of non-cospectral graphs with equal energy. These will be referred to as **A**-equienergetic.

The graph G is said to be hyperenergetic if its energy exceeds the energy of the complete graph K_n, or equivalently if $E(G) > 2n - 2$.

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A graph is called circulant if its adjacency matrix is circulant.

A graph is called integral if all eigenvalues of its adjacency matrix are integers.

So has characterized integral circulant graphs as follows. Let D be a set of positive, proper divisors of the integer $n > 1$. Define the graph $ICG_n(D)$ so that its vertex set be $Z_n = \{0, 1, \ldots, n-1\}$ and its edge set

$$\{\{a, b\} \mid a, b \in Z_n, \ \gcd(a-b, n) \in D\}.$$

- A class of integral circulant graphs is the generalization of well-known class of unitary Cayley graphs $ICG_n(1)$
- Integral circulant graphs are Cayley graphs of the additive group of Z_n and Cayley set S
- The graph $ICG_n(D)$ is regular of degree $\sum_{d \in D} \varphi(n/d)$, where $\varphi(n)$ denotes the Euler function
- These graphs are highly symmetric and have some remarkable properties connecting graph theory and number theory

$$D = \begin{pmatrix} 0 & 1 & 2 & 1 & 2 & 3 & 2 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 & 1 \\ 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 3 \\ 3 & 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 3 & 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 \\ 1 & 2 & 3 & 2 & 1 & 2 & 1 & 0 & 1 & 2 \\ 2 & 1 & 2 & 3 & 2 & 1 & 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 2 & 3 & 2 & 1 & 2 & 1 & 0 \end{pmatrix}$$

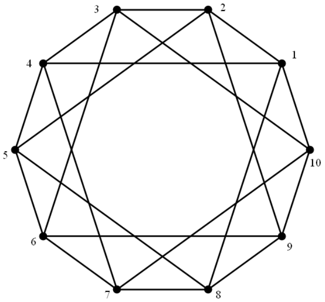

Figure: *The integral circulant graph $ICG_{10}(1)$ and its distance matrix.*

$$\lambda = \{-4, 4, -1, -1, -1, -1, 1, 1, 1, 1\} \qquad E(ICG_{10}(1)) = 16$$

$$\rho = \{15, -4, -4, -4, -4, 1, 0, 0, 0, 0\} \qquad DE(ICG_{10}(1)) = 32$$

$$\mu = \{8, 5, 5, 5, 5, 3, 3, 3, 3, 0\} \qquad LE(ICG_{10}(1)) = 16$$

Integral circulant graphs have found important applications:

- as a class of interconnection networks in parallel and distributed computing
- as potential candidates for modeling quantum spin networks that might enable the perfect state transfer (PST) between antipodal sites in a network
- in chemistry, as models for hyperenergetic and equienergetic graphs

Recently various graph parameters (such as diameter, clique number, chromatic number, automorphism group) were studied.

The Ramanujan function is defined as

$$c(j,n) = \sum_{\gcd(i,n)=1,\ 1\leq i<n} \omega_n^{ij}.$$

It is well-known from the number theory that

$$c(j,n) = \mu(t_{n,j})\frac{\varphi(n)}{\varphi(t_{n,j})}, \quad t_{n,j} = \frac{n}{\gcd(n,j)}$$

where μ is Möbius function.

Eigenvalues λ_j of integral circulants can be expressed using the Ramanujan function as follows:

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Eigenvalues λ_j of integral circulants can be expressed using the Ramanujan function as follows:

$$\lambda_j = \sum_{d \in D} c(j, n/d).$$

For arbitrary divisor d and $1 \leq i \leq n-1$, it holds

$$t_{n/d,i} = \frac{n/d}{\gcd(n/d, i)} = \frac{n}{\gcd(n, id)}$$

and

$$t_{n/d,n-i} = \frac{n/d}{\gcd(n/d, n-i)} = \frac{n}{\gcd(n, nd-id)}.$$

Since $\gcd(n, id) = \gcd(n, nd - id)$, we have $t_{n/d,i} = t_{n/d,n-i}$. Finally,

$$c(n/d, i) = \mu(t_{n/d,i}) \frac{\varphi(n/d)}{\varphi(t_{n/d,i})} = \mu(t_{n/d,n-i}) \frac{\varphi(n/d)}{\varphi(t_{n/d,n-i})} = c(n/d, n-i).$$

Therefore eigenvalues λ_i and λ_{n-i} are equal for $1 \leq i \leq n-1$.

The distance matrix of $ICG_n(D)$ is also circulant matrix and the distance spectrum of $ICG_n(D)$ is given by:

$$\rho_i = 1 \cdot \sum_{j=1}^{s_1} c\left(i, \frac{n}{d_j^{(1)}}\right) + 2 \cdot \sum_{j=1}^{s_2} c\left(i, \frac{n}{d_j^{(2)}}\right) + \cdots + diam(G) \cdot \sum_{j=1}^{s_{diam(G)}} c\left(i, \frac{n}{d_j^{(diam(G))}}\right)$$

where

$$D^{(p)} = \{d_1^{(p)}, d_2^{(p)}, \ldots, d_{s_p}^{(p)}\}\ ,\ 1 \leq p \leq diam(G)$$

is the set of divisors determined by the vertices on distance p from the starting vertex 0. Notice that $D^{(1)} = D$.

Theorem

The energy of unitary Cayley graph $ICG_n(1)$ equals $2^k\varphi(n)$, where k is the number of distinct prime factors dividing n.

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The distance energy of unitary Caley graph $ICG_n(1)$ equals

$$DE(ICG_n(1)) = \begin{cases} 2(n-1), & \text{if } n \text{ is a prime} \\ 4(n-2), & \text{if } n \text{ is a power of } 2 \\ 4n + 2\varphi(n)(2^{k-1}-1) - 2m & \\ -4 + 2\prod_{i=1}^{k}(2-p_i), & \text{if } n \text{ is odd composite number} \\ \frac{9n}{2} - 2m + 2\varphi(n)\cdot(2^k-3) & \\ -2 + \left|2(\varphi(n)-1) - \frac{n}{2}\right|, & \text{otherwise} \end{cases}$$

Let $n = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_k^{\alpha_k}$, where $p_1 < p_2 < \cdots < p_k$ are distinct primes, and $\alpha_i \geqslant 1$.

Lemma

If $k > 2$ or $k = 2$ and $p_1 > 2$, the following inequality holds

$$2^{k-1} \varphi(n) > n.$$

Corollary

The unitary Cayley graph $ICG_n(1)$ is hyperenergetic if and only if $k > 2$ or $k = 2$ and $p_1 > 2$.

Theorem

Let $n = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_k^{\alpha_k}$. For a two-element set of divisors $D = \{1, p\}$, the energy of the integral circulant graph $ICG_n(1, p)$ is given by

$$E(ICG_n(1,p)) = \begin{cases} 2^{k-1}(\varphi(n) + \varphi(n/p)), & p^2 \nmid n \\ 2^k(\varphi(n) + \varphi(n/p)), & p^2 \mid n \end{cases},$$

where p is a prime dividing n.

Theorem

Let n be a square-free number, $n = p_1 p_2 \cdots p_k$. Then the energy of integral circulant graph $ICG_n(p_i, p_j)$ does not depend on the choice of p_i and p_j,

$$E(ICG_n(p_i, p_j)) = 2^k \varphi(n) = 2^k \prod_{i=1}^{k} (p_i - 1).$$

We can construct at least k non-cospectral regular n-vertex hyperenergetic graphs,

$$ICG_n(1),\ ICG_n(p_1, p_2),\ ICG_n(p_1, p_3),\ \ldots,\ ICG_n(p_1, p_k),$$

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with equal energy.

Using a computer search on graphs with ≤ 10 vertices, we concluded that there are no pairs of **A**–, **L**–, and **D**– equienergetic graphs.

Let $n = 2pq$, where $p > q > 2$ are arbitrary prime numbers. Consider the following integral circulant graphs

$$G_n = ICG(2pq, \{1, 2\})$$

$$H_n = ICG(2pq, \{p, 2p, q, 2q\}).$$

We see that G_n and H_n are non-cospectral graphs with equal energy $8(p-1)(q-1)$, equal Laplacian energy $8(p-1)(q-1)$ and equal distance energy $4(3pq - 2p - 2q + 2)$.

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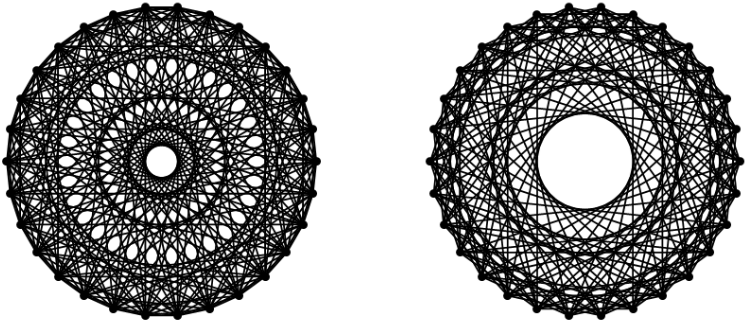

Figure: *A pair of triply equienergetic integral circulant graphs on 30 vertices H_{30} and G_{30}.*

Characterizing the set of positive numbers which can occur as energy of a graph has been a problem of interest.

Bapat proved that if the energy of a graph is rational then it must be an even integer.

Here we extend this result for the integral circulant graphs

Theorem

For odd n the energy of $ICG_n(D)$ is divisible by four.

Lemma

For $n \geq 2$ it holds that $c(j,n) \in 2N+1$ if and only if $4 \nmid n$ and $j = p_1^{\alpha_1 - 1} \cdots p_k^{\alpha_k - 1} J$ for some integer J such that $\gcd(J,n) \in \{1,2\}$.

$$E(G) = \lambda_0 + 2 \sum_{i=1}^{(n-1)/2} |\lambda_i|$$

Since $x \equiv |x| \pmod 2$, we have

$$\frac{E(G)}{2} \equiv \sum_{d \in D} \frac{\varphi(n/d)}{2} + \sum_{i=1}^{(n-1)/2} \sum_{d \in D} c(i, n/d) \pmod 2.$$

After exchanging the order of the summation

$$\frac{E(G)}{2} \equiv \sum_{d \in D} \frac{\varphi(n/d)}{2} + \sum_{d \in D} \sum_{i=1}^{(n-1)/2} c(i, n/d) \pmod 2.$$

Using the largest square-free divisor of n/d we finally get

$$\frac{E(G)}{2} \equiv \sum_{d \in D} \frac{d+1}{2} \varphi(n/d) \pmod 2.$$

Since n is odd, $d/2 \notin D$ and therefore $\varphi(n/d)$ is even for any $d \in D$.

Questions for the further research:

- It would be interesting to calculate the energy of an arbitrary integral circulant graph $X_n(D)$
- Characterize the structure of divisor sets D producing integral circulant graphs with minimal/maximal energy for fixed value n
- Analyze other graph-theoretical properties of integral circulant graphs

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Thank you!