A STUDY ON ENERGY OF GRAPH

Project report submitted to Christ College (Autonomous) in partial fulfilment of the requirement for the award of the M.Sc Degree programme in Mathematics

by

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2021

CERTIFICATE

This is to certify that the project entitled **"A STUDY ON ENERGY OF GRAPH"** submitted to Department of Mathematics in partial fulfilment of the requirement for the award of the M.Sc Degree programme in Mathematics, is a bonafide record of original research work done by **Ms. AMRITHA K S (CCATMMS003)** during the period of her study in the Department of Mathematics, Christ College (Autonomous), Irinjalakuda, under my supervision and guidance during the year 2020-2021

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Place : Irinjalakuda

Date : 31 March 2021

DECLARATION

I hereby declare that the project work entitled "**A STUDY ON ENERGY GRAPH**" submitted to Christ College(Autonomous), Irinjalakuda in partial fulfilment of the requirement for the award of Master Degree of Science in Mathematics is a record of original project work done by me during the period of my study in the Department of Mathematics, Christ College(Autonomous), Irinjalakuda.

Place : Irinjalakuda **AMRITHA K S**

Date : 31 March 2021

ACKNOWLEDGEMENT

First, there are no words to adequately acknowledge the wonderful grace that my Redeemer has given me. There are many individuals who have come together to make this project a reality. I greatly appreciate the inspiration; support and guidance of all those people who have been instrumental for making this project a success.

I express my deepest thanks to my guide Dr. Joju K T, Associate Professor(Rtd), Department of Mathematics, Christ College(Autonomous), Irinjalakuda, who guided me faithfully through this entire project. I have learned so much from her, both in the subject and otherwise. Without her advice, support and guidance, it find difficult to complete this work.

I take this opportunity to express my thanks to our beloved principal Fr. Dr. Jolly Andrews CMI, who gave me the golden opportunity to do this wonderful project on the topic "**A STUDY ON ENERGY GRAPH**"

I mark my word of gratitude to Prof. Tintumol Sunny, Head of the Department and all other teachers of the department for providing me the necessary facilities to complete this project on time.

My project guide Dr. Joju K T, deserves a special word of thanks for her invaluable and generous help in preparing this project in LAT_EX.

I want to especially thank all the faculty of the library for providing various facilities for this project.

Words cannot express the love and support I have received from my parents, whose encouragement has buoyed me up from the beginning till the end of this work.

AMRITHA K S

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Introduction

The basics idea of graph theory were born in 1736 with Euler's paper in which he solved the Konigsberg bridge problem.In the last decades graph theory has established itself as a worthwhile mathematical disciplines and there are many applications of graph theory to a wide variety of subjects which include operation research, Physics, Chemistry, Economics, Genetics, Sociology, Engineering etc. We can associate several matrices which record information about vertices and how they interconnected. That is we can given an algebraic structure to every graph.Many interesting result can be proved about graphs using matrices and other algebraic properties. The main use of algebraic structure is that we can translate properties of graphs into algebraic properties and then using the results and methods of algebra, to deduce theorems about graphs.

We mainly concendrate on Eigenvalues of the adjacency matrices of some graphs. In early days, important progress was made in the development of algebraic theory by the investigation of some very concrete problems, for example, Kirchoffs study of electrical circuits and cayleys attempt to enumerates chemical isomers.

Application of matrices are not only graph theory. There are many ideas applied in field of secret in the banking, communication in military administration,confidential message transduction, computerized lockers etc.

Outline of the Project

Apart from the introductory chapter, We have described our work in three chapters.

Chapter 1: In this chapter we review the basic concepts in graph theory and linear algebra. In graph theory section we review some definitions [1] and notations and In the linear algebra section we review some useful results in matrix theory.

Chapter 2: This chapter begins by defining matrices associated with graphs.We shall restrict our attention to simple undirected graphs. So whenever the word graph is used it will be referring to simple undirected graph with n vertices.

chapter 3: In this chapter we discuss about energy of graph.

Chapter 4: This chapter shown that there exist an infinite number of values of n for which k-regular graphs exist whose energies are arbitrarily small compared to the known sharp bound $k + \sqrt{k(n-1)(n-k)}$ for the energy of k-regular graphs on n vertices.

Chapter 1

preliminaries

1.1 Graphs

Definition 1.1.1. A Graph G is a non empty set of vertices $V(G)$ and a set of edges $E(G)$ which consist of pair of elements of $V(G)$ [1].

(1) The graph G is said to be directed graph(diagraph) if elements of $E(G)$ are ordered pairs and undirected if they are not.

(2) If $\{v_i, v_j\} \in E(G)$, then v_i is said to be adjacent to v_j.

(3) If an edge joints a vertex to itself such an edge is known as loop.

(4) If some pair of vertices are connected by more than one edge, such edges are called parallel edges.

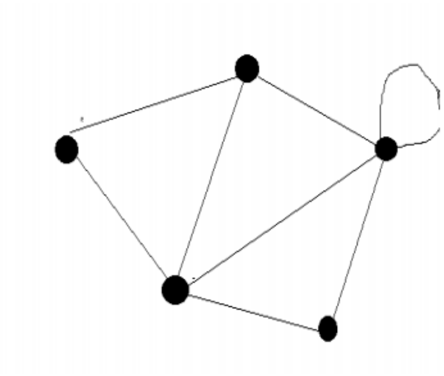

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Figure 1.1: A graph with multiple edges and loop

Definition 1.1.2. A graph G is simple if it has no loops and parallel edges.

Definition 1.1.3. If a graph G contains some loops or parallel edges then G is called multi graph.

Definition 1.1.4. The degree of vertex in a simple graph G is the number of edges incident with v.

A graph in which every vertex has equal degree K is called regular of degree K or K-regular.

Definition 1.1.5. A subgraph of a graph H such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ and the assignment of end points to edges in H is same as in G.

Definition 1.1.6. A path p_n is a graph with n vertices and edges set $\{v_i, v_{i+1} : 1 \leq i < n\}$.

Definition 1.1.7. A graph G is said to be connected if there is a path between every two of its vertices.

Definition 1.1.8. A cycle is a path in which all the vertices except the end vertices are disjoint.

Some special graphs

- A simple graph in which every pair of distinct vertices are adjacent is called a complete graph. A complete graph of n-vertices is denoted by k_n.

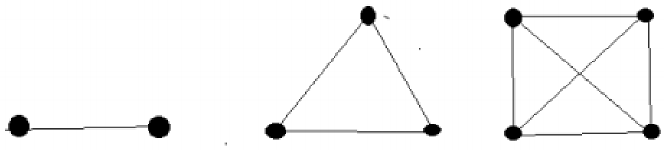

Figure 1.2: complete graph

- A cycle graph of order n is a connected graph of n-vertices whose edges form a cycle of length n and is denoted by c_n.

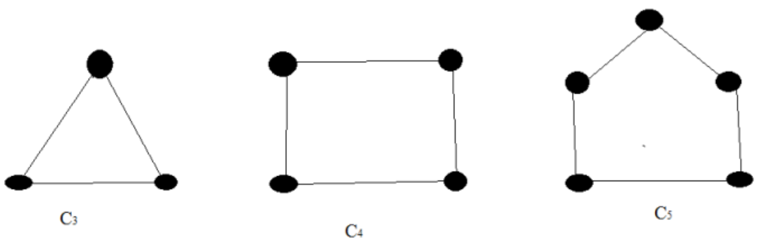

Figure 1.3: Example of a cycle

- A bipartite graph is a simple undirected graph whose vertex set V can be partitioned into two sets M and N in such a way that each edge joints a vertex M to a vertex in N and no edge joins either two vertices in M or two vertice in N. Example of a bipartite graph is given below.

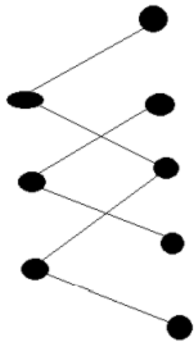

Figure 1.4: An example of a bipartite graph

- A bipartite graph in which every vertex in M is adjacent with every vertex in N is known as complete bipartite graph.A complete bipartite graph is denoted by $k_{m,n}$.

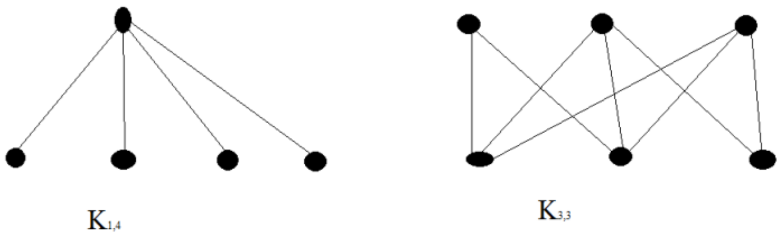

Figure 1.5: Example of a complete bipartite graph

Graph isomorphism

there are different ways to draw the same graph [1]. Consider following pair of graphs.

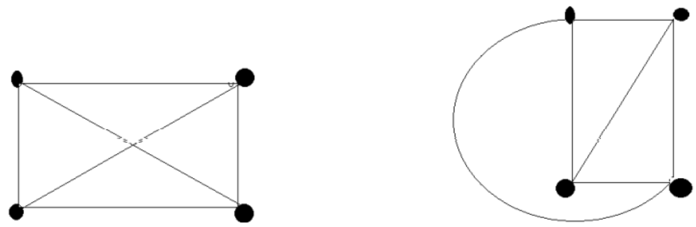

Figure 1.6: Pair of isomorphic graphs

Definition 1.1.9. Graph $G_1(V_1, E_1)$ and $G_2(V_2, E_2)$ are isomorphic if there is a bijection $f\colon V_1 \to V_2$ and There is a bijection $g\colon E_1 \to E_2$ such that u and v are adjacent in G_1 if and only if $f(u)$ and $f(v)$ are adjacent to G_2.

Example of non-isomorphic graph is given in figure 1.7

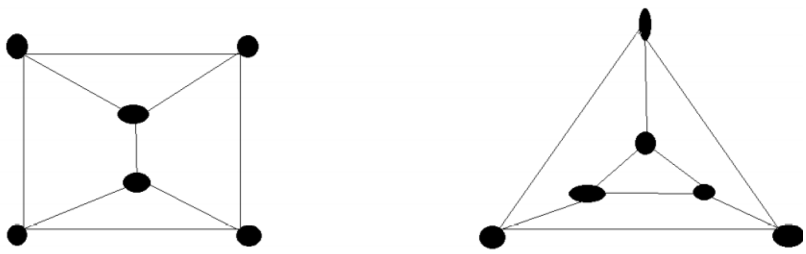

Figure 1.7: Non-isomorphic graphs

1.2 Linear algebra

Matrices

A matrix A over a field K or, simply a matrix A is a rectangular array of $m \times n$ matrix consists of mn real numbers arranged in m rows and n columns. The entry in row i and column j of a matrix A is denoted by $a_{i,j}$. An $m \times 1$ matrix is called a column vector of order m. Similarly, a $1 \times n$ matrix is a row vector of order n. An $m \times n$ matrix is called a square matrix if $m = n$. A diagonal matrix is a square matrix A such that $a_{i,j} = 0; i \neq j$. We denote the diagonal matrix by diag$(\lambda_1, \lambda_2, ..\lambda_n)$. when $\lambda_i = 1$ for all i, this matrix reduces to the identity matrix of order n, which is denoted by I_n.

Trace

Let A be a square matrix of order n. The entries $a_{11}, a_{22}, ...a_{nn}$ are the main diagonal of A. The trace of A is defined as $Trace(A) = a_{11}+, a_{22}, ...a_{nn}$

Example 1.2.1.

$$A = \begin{bmatrix} 2 & 2 & -4 \\ -1 & 1 & 3 \\ 2 & 0 & -1 \end{bmatrix}$$

$Trace(A) = 2 + 1 + -1 = 2$

Eigenvalues of symmetric matrices

Let A be a $n \times n$ matrix . The determinant $det(A - \lambda I)$ is a polynomial in the (complex) variable λ of degree n and is called the characteristic polynomials of A . The equation $det(A - \lambda I) = 0$ is called the characteristic equation of A. By fundamental theorem of algebra the equation as n complex roots and this roots are called Eigen value.

Chapter 2

Matrices Associated With Graphs

2.1 Adjacency matrix

In this section we introduce the concept of adjacency matrix [3] of graph. We also discuss some properties of adjacency matrix.

Definition 2.1.1. Let G be a graph with $V(G) = \{v_1, v_2 ...., v_n\}$ and $E(G) = \{e_1, e_2, ...e_m\}$ the **Adjacency matrix of G**, denoted by $A(G)$, is the $n \times n$ matrix defined as follows,

$$a_{i,j} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

We often denote A(G) by A

Example 2.1.1. Consider the graph G in figure 2.1

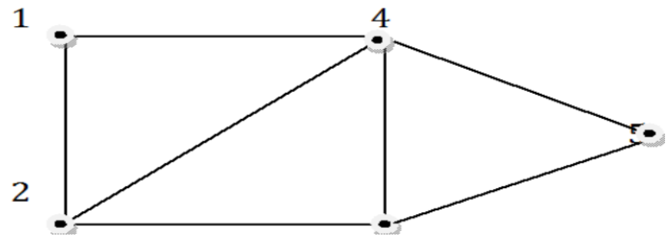

Figure 2.1: Graph G (a)

$$\text{Then, } A(G) = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

Properties of adjacency matrix

Let A(G) be an adjacency matrix, then

(1) Elements of the diagonal entry of A(G) are zeroes.

(2) A is real symmetric matrix.

(3) Sum of entries in the i th row is the degree of the vertex.

(4) A is diagonalizable.

(5) Eigen value of A(G) are real

Lemma 2.1.1. Two graphs are isomorphic if and only if for some ordering of their vertices their adjacency matrices are equal.

Theorem 2.1.1. Let G be a graph and A(G) be the adjacency matrix of G. Then

1. Sum of the 1×1 principal minor of A is zero.
2. Sum of the 2×2 principal minor of A is equal to the number of edges of G.
3. Sum of the 3×3 principal minor of A is equal to twice the number of triangles in G

Proof. 1. The principle minor with one row and column is the corresponding diagonal entry. This implies that sum of the 1×1 principle minor of A is zero.

2. A principle minor with two row and columns, and which as a non zero entry, must be the form $\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$
   There is one such minor for each pair of adjacency vertices of G, and each has value -1. That is sum of principal minor of A of order two = $|E(G)| \times -1 = -|E(G)|$, giving the result.

3. There are essentially three possibilities for non trivial principal minor with three rows and columns. $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$ and of these, the only nonzero one is the whose value is 2. This principal minor corresponds to three mutually adjoint vertices in G. That is corresponds to the triangle in G.

□

2.2 Incident matrix

In this section we introduce the concept of incidence matrix of a graph. In mathematics incidence matrix is a matrix that shows relationship between two classes of objects . If the 1st class is X and 2nd class is Y. The matrix has one row for each element of X and one column for each element of Y. The entry in row x and column y is 1 if x and y are related and 0 if they are not. Incidence matrix are mostly used in graph theory.

Definition 2.2.1. Let G be a graph with $V(G) = \{v_1, v_2, ..., v_n\}$ and $E(G) = \{e_1, e_2, ...e_n\}$. The **Incident matrix** $Q = Q(G)$ of G is $n \times m$ matrix whose entries $q_{i,j}$ are given by

$$q_{i,j} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are incident} \\ 0 & \text{otherwise} \end{cases}$$

Example 2.2.1.

Figure 2.2: Graph G_1 and G_2

The incident matrix of G_1

$$Q(G_1) = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

The incident matrix of G_2 is

$$Q(G_2) = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Note that the incident matrix contains only two types of element 0 and 1. This clearly is a binary matrix of $(0, 1)$

We have the following informations about the incident matrix Q(G):

(1) Since every edge is incident exactly two vertices, each column of Q(G) has exactly two one's.

(2) The number of one's in each row equals the degree of the corresponding vertex.

(3) A row with all zeroes represents an isolated vertex.

(4) Parallel edges in a graph produce identical columns in the incidence matrix.

(5) If a graph is disconnected and consists of two components G_1 and G_2, the

incidence matrix Q(G) of the graph G can be written in a diagonal form as

$$Q(G) = \begin{bmatrix} Q(G_1) & 0 \\ 0 & Q(G_2) \end{bmatrix}$$

where $Q(G_1)$ and $Q(G_2)$ are the incidence matrices of componentsG_1 and G_2.

(6) Permutation of any two rows or columns in an incident matrix simply corresponds to relabeling the vertices and edges of the same graph

Definition 2.2.2. Let G is an oriented graph. The **directed incidence matrix** of G is the $n \times m$ matrix $Q = Q(G)$ whose entries $q_{i,j}$ are given by

$$q_{i,j} = \begin{cases} 1 & \text{if } v_i \text{ is the positive end of } e_j \\ -1 & \text{if } v_i \text{ is the negative end of } e_j \\ 0 & \text{otherwise} \end{cases}$$

The rows of directed incidence matrix corresponds to the vertices of G_1 and its columns corresponds to the edges of G. Each column contains only two nonzero entries +1 and -1. The number of non zero entries in the i th row is the degree of the vertex v_i.

Example 2.2.2. Consider the oriented graph G in figure 2.3 with $V = \{v_1, v_2, v_3, v_4\}$ and $E = \{e_1, e_2, e_3, e_4, e_5\}$

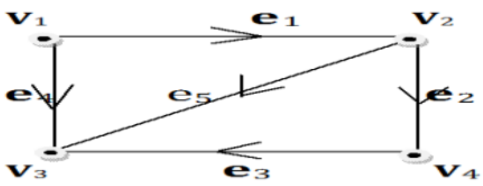

Figure 2.3: Example of an oriented graph

The incidence matrix is given by

$$Q(G) = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 \end{bmatrix}$$

2.3 Degree matrix

Definition 2.3.1. Let G be a graph. **The Degree matrix of G** is $n \times n$ matrix $\Delta = \Delta(G)$ having $\delta_{i,j} = deg(v_i)$

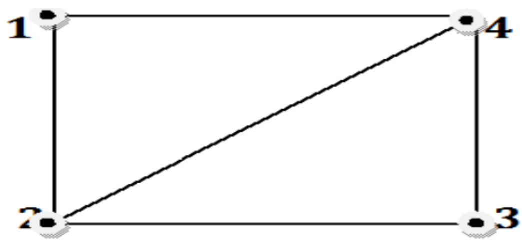

Figure 2.4: Graph G (b)

Example 2.3.1. Degree matrix of Graph G (b) is

$$\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

2.4 Laplacian matrix

Definition 2.4.1. Let G be a graph with $V(G) = \{v_1, v_2, ..., v_n\}$ and $E(G) = \{e_1, e_2, ...e_m\}$. The Lapacian matrix of G is the $n \times n$ matrix whose entries $l_{i,j}$ are defined as follows,

$$l_{i,j} = \begin{cases} d_i & \text{if } i = j \\ -1 & v_i \text{ Adjacent } v_j \\ 0 & \text{otherwise} \end{cases}$$

The Laplacian matrix is denoted by L(G).

Example 2.4.1. Consider figure 2.5,

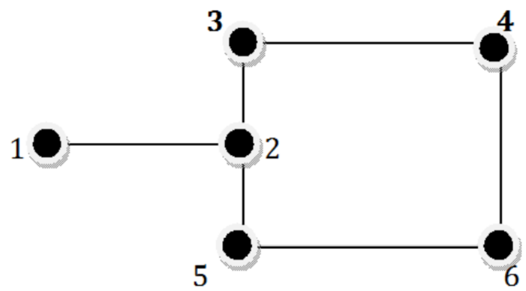

Figure 2.5: A graph with 5 vertices and 6 edges

$$A(G) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

$$\Delta(G) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

$$L(G) = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & 0 & -1 \\ 0 & -1 & 0 & 0 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

- The diagonal entries of $L(G)$ are the degree of the corresonding vertex and note that $L(G) = \Delta(G) - A(G)$.

- Laplacian matrix is also known as Kirchoff matrix.

Given any orientation to the edges,label the edges. The vertex edge incidence matrix Q.

$$q_{i,j} = \begin{cases} +1 & \text{if } v_i \text{ is the positive end of } e_j \\ -1 & \text{if } v_i \text{ is the negative end of } e_j \\ 0 & \text{otherwise} \end{cases}$$

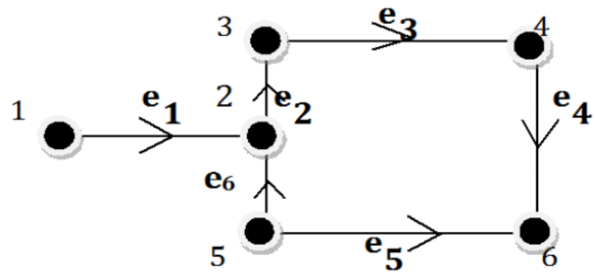

Figure 2.6: Oriented graph with 6 vertices and 6 edges

For this graph we have

$$Q(G) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & -1 & -1 & 0 \end{bmatrix}$$

Then observe that $Q(G).Q(G)^T = L(G)$.

Lemma 2.4.1. Let G be a graph with $V(G) = v_1, v_2, ...v_n$ and $E(G) = e_1, e_2, ...e_n$. Then the following sections hold.

1. L(G) is a symmetric, positive semi definite matrix.

2. The rank of $L(G)$ equals $n - k$, where k is the number of connected components of G

3. For any vector x, $x'L(G)x = \sum_{i,j}(x_i - x_j)^2$

4. The row sum and column sum of $L(G)$ are zero.

Proof. 1. It is obvious from $L(G) = Q(G).Q(G)'$ that $L(G)$ is symmetric and positive semidefinite. since,

$$\begin{aligned} detL(G) &= detQ(G)detQ(G)^{'} \\ &= detQ(G)detQ(G) \\ &= detQ(G)^2 \\ &\geq 0 \end{aligned}$$

and

$$\begin{aligned} L(G)^T &= (Q(G).Q(G)^{'})^{'} \\ &= (Q(G)^{'})^{'}.Q(G)^{'} \\ &= Q(G)Q(G)^{'} \end{aligned}$$

2. Observe that,

$$rank(G) = (rankQ(G).Q(G)^{'})$$

$$min\{rankQ(G), rankQ(G)^{'}\} = rankQ(G)$$

$$= n - k$$

3. $x^{'}L(G)x = x^{'}Q(G)Q(G)^{'}x$

   The vector $x^{'}Q(G)$ is indexed by the edge $e = \{i, j\}$ is (x_i, x_j).

   Hence $x^{'}Q(G)Q(G)^{'}x = (x_i, x_j)(x_i, x_j) = (x_i, x_j)^2$

4. This follows from the definition $L(G) = \Delta(G) - A(G)$.

$\square$

Chapter 3

The Energy Of Graph

3.1 Energy of graph

The energy E(G) of a graph G is defined to be the sum of the absolute values of Eigen values of G. Hence if A(G) is the adjacency matrix of G and $\lambda_1, \lambda_2, ..., \lambda_n$ are Eigen values of A(G) then

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

As the sum of the absolute values of Eigen values . The energy of any graph G, E(G) is always greater than or equal to zero. Since for the totaly disconnected graph K_n^c is the adjacency matrix is a zero matrix. There for it has no nonzero Eigen values. Thus the energy of totally disconnected graph is zero [2] that is $E(K_n^c) = 0$ and thus zero is connected as the lower bound for graph energy.

Example 3.1.1. The complete graph K_n has energy $2(n-1)$.

We have Eigen values of K_n are $n-1$ and $-1,-1,.....-1\{n-1\ times\}$ There for

$$
\begin{aligned}
E(G) &= \sum_{i=1}^{n} |\lambda_i| \\
&= (n-1)+1+1+1+....+1 \\
&= 2(n-1)
\end{aligned}
$$

Result 1. Energy of a disconnected graph is the sum of the energies of its connected.

Proof. Let G be a disconnected graph with n components. Let $G_1, G_2, ...G_n$ be its components and let A(G) be the adjacency matrix of G. Construct the vertex set V of G as by considering the vertices of the component G_1 first and followed by the vertices of G_2 and then vertices of G_3 and follow like this and consider the vertices of G_n at last.

If $A(G_1), A(G_2), ...A(G_n)$ are adjacency matrixes of $G_1, G_2, ...G_n$ respectively and 0 represents the matrix of all entries zero, then $A(G)$ has the following form

$$
A(G) = \begin{bmatrix}
A(G_1) & 0 & 0 & \dots & 0 & 0 \\
0 & A(G_2) & 0 & \dots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \dots & A(G_{n-1}) & 0 \\
0 & 0 & 0 & \dots & 0 & A(G_n)
\end{bmatrix}
$$

Then by a theorem from matrix theory, we have the Eigen values of A(G) is same as the union of the Eigen values of the components $A(G_1), A(G_2), ...A(G_n)$. Let K_j is the order of the component G_j and let $\lambda_{i,1}, \lambda_{i,2}, ...\lambda_{i,n}(i.e., \lambda_{i,j}, i = 1, 2, ...k_j)$are the Eigen values of G are given by,

$\{\lambda_{i,j} : i = 1, 2, 3, ...k_j \ and \ \ j = 1, 2, ...n\}$. Thus

$$\begin{aligned} E(G) &= \sum_I \sum_J |\lambda_{i,j}| \\ &= \sum_J E(G_J) \end{aligned}$$

That is $E(G) = E(G_1) + E(G_2) + ... + E(G_n)$. Thus we can conclude that "the energy of a graph G is same as the sum of the energies of its connected components". □

Result 2. for a simple graph G with Eigen values $\lambda_1, \lambda_2, ...\lambda_n$, we have

$$\sum\{\lambda_i : \lambda_i > 0\} = \sum\{\lambda_i : \lambda_i < 0\} = \frac{1}{2}E(G)$$

Proof. Let G be a simple graph having n vertices and m edges. Let A(G) be the adjacency matrix of G, and let $\lambda_1, \lambda_2, ...\lambda_n$ are Eigen values of G. Since the adjacency matrix of a simple graph is symmetric matrix having zeroes on the diagonal. We have sum of its diagonals is again zero.

That is $trace\ A = 0$. But we have ,

$$\begin{aligned} &\sum_{i=1}^{n} \lambda_i = trace\ A \\ &\implies \sum_{i=1}^{n} \lambda_i = 0 \\ &\implies \sum\{\lambda_i : \lambda_i > 0\} + \sum\{\lambda_i : \lambda_i < 0\} = 0 \end{aligned}$$

$$\Longrightarrow \sum\{\lambda_i : \lambda_i > 0\} = -\sum\{\lambda_i : \lambda_i < 0\} \qquad (1)$$

$$\begin{aligned} Now \quad E(G) &= \sum |\lambda_i| \\ &= \sum\{|\lambda_i| : \lambda_i > 0\} + \sum\{|\lambda_i| : \lambda_i < 0\} \\ &= \sum\{\lambda_i : \lambda_i > 0\} - \sum\{\lambda_i : \lambda_i < 0\} \\ &= 2\sum\{\lambda_i : \lambda_i > 0\} \end{aligned}$$

Therefor $\quad \sum\{\lambda_i : \lambda_i > 0\} = \frac{1}{2}E(G)$

Therefore by (1) we can conclude that

$-\sum\{\lambda_i : \lambda_i < 0\} = \sum\{\lambda_i : \lambda_i > 0\} = \frac{1}{2}E(G)$

In graph theory there is a result that showing bounds of Eigen values of G. “Let λ be an Eigen value of a graph G with n vertices and m edges, then

$$|\lambda_i| \leq \sqrt{\frac{2m(n-1)}{n}}$$

From this we shall obtain the following result. □

Result 3. Let G be a simple graph with n vertices and m edges and having Eigen values $\lambda_1, \lambda_2, ...\lambda_n$ then,

$$E(G) \leq \sqrt{2mn(n-1)}$$

Proof. By the above result we have,

$$|\lambda_i| \leq \sqrt{\frac{2m(n-1)}{n}} \qquad \forall\ i = 1, 2, ...n$$

Therefore,

$$\begin{aligned}
E(G) &= \sum_{i=1}^{n} |\lambda_i| \\
&\leq \sum_{i=1}^{n} \sqrt{\frac{2m(n-1)}{n}} \\
&\leq n \times \sqrt{\frac{2m(n-1)}{n}} \\
&= \sqrt{2mn(n-1)}
\end{aligned}$$

That is, $E(G) \leq \sqrt{2mn(n-1}$ □

3.2 Hyper-energitic and Non-hyper-energitic graph

Since the complete graph Kn, the graph with the maximum possible number of edges (among graph on n vertices) has energy $2(n-1)$. **I.Gutman** (in 1978)conjectured in the paper [6] that "All graphs have energy atmost $2(n-1)$". But then this was disproved by Chris Godsil, by introducing an n vertex graph having energy greater than $2(n-1)$.

Definition 3.2.1. A graph G having energy greater than the energy of the complete graph on the same number of vertices is called a **hyper energetic graph**. That is if for a graph in n vertices $E(G) > 2(n-1)$ then G is called a hyper energetic graph.

Definition 3.2.2. A graph G having energy less than or equal to the energy of the complete graph on the same number of vertices is called **non hyper-**

energetic graph. That is G is an n vertex graph and if $E(G) \leq 2(n-1)$, then G is called a non hyperenergetic graph. A **Circulant matrix** is a special kind of Toeplitz matrix (matrices with constant diagonals are called Toeplitz matrices) where each row vector is rotated one element to the right relative to the preceding row vector.An $n \times n$ Circulant matrix C takes the form,

$$C = \begin{bmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \iddots & c_2 \\ \vdots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & \ddots & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{bmatrix}$$

A Circulant matrix is fully specified by one vector, c, which appears as the first column of C. The remaining columns of C are each cyclic permutations of the vector c with offset equal to the column index. The last row of C is the vector c in reverse order, and the remaining rows are each cyclic permutations of the last row.

Note that difference source define circulant matrix in different way, for example with the coefficients corresponding to the first row rather than the first column of the matrix, or with a different direction of shift. The Eigen values of a Circulant matrix are given by $\lambda_j = c_0 + c_{n-1}\omega_j + c_{n-2}\omega_j^2 + ... + c_1\omega_j^{n-1}, \quad j = 0, ...n-1$ Where ω_j are the n th roots of unity and $i = \sqrt{-1}$ is the imaginary unit.

Lemma 3.2.1. If C is a Circulant matrix of order n with first row $a_1, a_2, ...a_n$ then the determinant of C is given by,

$detC = \prod_{0\leq j\leq n-1} a_1 + a_2\omega^j + a_3\omega^{2j} + ... + a_n\omega^{(n-1)j}$, where ω is the primitive n th root of unity.

3.3 Circulant graph

Let $S \subset 1, 2, \ldots, n$ with the property that if $i \in S$ then $n - i \in S$. The graph G with the vertex set $V = \{v_0, v_1, ...v_{n-1}\}$ in which v_i adjacent to v_j if and only if $i - j(modn) \in S$, is called a circulant graph of order n.

Since the adjacency matrix $A(G)$ of G is a Circulant matrix of order n with 1 in the $(i + 1)$ th position of its first row if and only if $i \in S$ and zero in the remaining positions.

Clearly G is a $|S|$ regular graph, if $S = \{\alpha_1, \alpha_2, ...\alpha_n\}$ a subset of $\{1, 2, \ldots, n\}$ then first row of $A(G)$ poses 1 in the $(\alpha_i + 1)$ th position for $1 \leq i \leq k$ and zero in the remaining positions. Hence by above lemma, the Eigen values are given by $\{\omega^{j\alpha_1} + \omega^{j\alpha_2} + ...\omega^{j\alpha_k} : 0 \leq j \leq n - 1, w = a$ primitive n th root of unity$\}$.

Definition 3.3.1. A Hamilton graph is a graph with a spanning cycle, it is also called a **Hamilton cycle**.

Example of non hyper energetic graph

Example 3.3.1. All graph of order n with number of edges less than $2n - 2$ are non hyper-energetic

Definition 3.3.2. A subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex on each edge of G. Hence if G has n vertices and m edges then its subdivision graph $S(G)$ has $m + n$ vertices and $2m$ edges.

Example 3.3.2. All subdivision graphs are non-hyperenergetic. Recall that the subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex on each edges of G.

Hence if G has n vertices and m edges,$S(G)$ has $m + n$ vertices and $2m$ edges. Now all graphs of order n with number of edges less than $2n - 2$ are non-hyper-energetic.For all subdivision graph of non-trivial graph, we have

$$2m < 2|V(S(G))| - 2 = 2(m + n) - 2$$

Hence all subdivision graphs are non-hyperenergetic

Chapter 4

Energy Bounds

For a graph G on n vertices and having m edges, it's shown in the research paper [6] that

$$E(G) \leq \frac{2m}{n} + \sqrt{n - 1 \left[2m - \left(\frac{2m}{n}\right)^2\right]} = B_1 \tag{4.1}$$

Now consider a k-regular graph, then we have the number of edges of this k-regular graph is $m = \frac{nk}{2}$, apply this in the above equation, then we will get

$$\begin{aligned} E(G) &\leq \frac{2\frac{nk}{2}}{n} + \sqrt{(n-1)\left[2\frac{nk}{2} - \left(\frac{2(\frac{nk}{2})}{n}\right)^2\right]} \\ &= \frac{2nk}{2n} + \sqrt{(n-1)\left[\left(\frac{2nk}{2}\right) - \left(\frac{2nk}{2n}\right)^2\right]} \\ &= k + \sqrt{(n-1)(nk - k^2)} = B_2 \;\; (say) \end{aligned} \tag{4.2}$$

This is for a k-regular graph G of order n, $E(G) \leq k + \sqrt{k(n-1)(n-k)} = B_2$

4.1 Cubic Graph

Definition 4.1.1. **Cubic graph** is a graph that is a regular of degree 3.

from (4.2) and this definition, we shall obtain the following result.

Result 4. All cubic graphs are non hyper-energitic.

Proof. We know that a cubic graph is a 3-regular graph. Now consider the upper energy bound $B_2 = k + \sqrt{k(n-1)(n-k)}$ of a k-regular graph and put $k = 3$, $B_2 = 3 + \sqrt{3(n-1)(n-3)}$

Now,

$$\begin{aligned} B_2 &\leq 2(n-1) \qquad (4.3) \\ \Rightarrow 3 + \sqrt{3(n-1)(n-3)} &\leq 2(n-1) \\ \Rightarrow \sqrt{3(n-1)(n-3)} &\leq 2n - 5 \\ \Rightarrow 3(n-1)(n-3) &\leq (2n-5)^2 \\ \Rightarrow 3(n^2 - 4n + 3) &\leq 4n^2 - 20n + 25 \\ \Rightarrow 0 &\leq n^2 - 8n + 16 \\ \Rightarrow 0 &\leq (n-4)^2 \qquad (4.4) \end{aligned}$$

Now since (4.4) is true, we get that (4.3) is also true that is $B_2 \leq 2(n-1)$. So $E(G) \leq B_2 \leq 2(n-1)$ this implies that G is non hyper energitic. Therefore we can conclude that every cubic graph is non hyper-energitic. □

Note: There are regular for which the bound B_2 is attained.

To see this, consider the complete graph K_n, clearly K_n is a $(n-1)$ regular graph.so

$$\begin{aligned}B_2 &= k+\sqrt{k(n-1)(n-k)}\\ &= (n-1)+\sqrt{(n-1)(n-2)(n-(n-1))}\\ &= (n-1)+(n-1)\\ &= 2(n-1)\end{aligned}$$

Also we have $E(K_n) = 2(n-1)$. i.e, we got that $E(K_n) = B_2$. Showing that both B_1 and B_2 are sharp bound for the energy concept of a simple graph.

Lemma 4.1.1. For any two positive integer n and $k, n-1 > k \geq 2$ and $\epsilon > 0$, does there exist a k-regular graph G with $\frac{E(G)}{B_2} > 1-\epsilon$, where $B_2 = k+\sqrt{k(n-1)(n-k)}$

Proof. We know $E(G) \leq B_2$. For $\epsilon > 0$ we can write $E(G)+\epsilon = B_2$. By the condition $n-1 > k \geq 2$, it is clear B_2 always greater than 1. Then $E(G)+\epsilon > 1$

$$\begin{aligned}&E(G) > 1-\epsilon\\ &\implies \frac{E(G)}{B_2} > 1 > \frac{1-\epsilon}{B_2}\end{aligned}$$

As $B_2 > 1$

$$\implies \frac{E(G)}{B_2} > 1-\epsilon$$

□

Recently J. H. Koolen and V. Moulton in papers maximal energy graphs [8] and maximal energy bipartite graph [7] showed that for a graph G with n vertices and m edges

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)(2m - \frac{4m^2}{n^2})} \tag{4.5}$$

And for bipartite graph with n vertices and m edges

$$E(G) \leq \frac{4m}{n} + \sqrt{(n-2)(2m - \frac{4m^2}{n^2})}$$

And characterized those graphs for which these bounds are best possible. Then they proved that for graph G with n vertices

$$E(G) \leq \frac{n}{2}(\sqrt{n} + 1)$$

And for bipartite graph G with n vertices

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n} + \sqrt{2})$$

And those graphs for which these bounds are best possible can be characterized.

4.2 Semi regular bipartite Graph

Definition 4.2.1. A graph G is **semi regular bipartite** (of degree r_1 and r_2) if it is bipartite and each in the same part of bipartition has the same degree (each vertex in one part of bipartition has degree r_1 and each vertex in the other part of bipartition has degree r_2)

Clearly a regular bipartite graph is a semi-regular bipartite graph with $r_1 = r_2$
If $\lambda_1 \geq \lambda_2 \geq .... \geq \lambda_n$ eigen values of G among the known lower bounds of λ_1 [5] is the following

$$\lambda_1 \geq \sqrt{\frac{\sum_i d_i^2}{n}} \tag{4.6}$$

And the equality holds if and only if G is a regular bipartite graph, where $d_1, d_2, ..., d_n$ the degree sequence of G. The degree sequence of a graph G is the list of vertex degrees, usually written in non increasing order, as $d_1 \geq d_2 \geq ... \geq d_n$

4.3 Strongly regular Graph

Definition 4.3.1. A **strongly regular graph**G with parameters (n, k, ρ, σ) is a k-regular graph on n vertices each pair of adjacent vertices has ρ common neighbors and each pair of non adjacent vertices has σ common neighbors.
If $\sigma = 0$, then G is a disjoint union of complete graph, whereas if $\sigma \geq 1$ and G is non-complete, then the Eigen values of G are k, s and t with multiplicities 1, m_s and m_t where s, t are the root $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$, this because a theorem from graph theory. A k-regular connected graph G is strongly regular with parameters n, k, ρ, σ and only if it has exactly 3 Eigen values k, s and t such that $k > s > t$ and these satisfies $s + t = \rho - \sigma$ and $st = \rho - k$. i.e s, t are roots of $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$ and m_s and m_t are determined by $m_s + m_t = n - 1$ (sum of the multiplicities of Eigen values of a graph G is the order of G) and $k + m_s s + m_t t = 0$ (sum of the Eigen values of a simple graph = trace A = 0).

Theorem 4.3.1. If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, ...d_n$ then,

$$E(G) \leq \sqrt{\frac{\sum_i d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_i d_i^2}{n}\right)} \tag{4.7}$$

Moreover the equality holds if and only if G either

1. $\frac{n}{2}K_2 \quad (m = \frac{n}{2})$
2. $K_n \quad (m = \frac{n(n-1)}{2})$
3. A non-complete connected strongly regular graph with two non trivial Eigen values both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$, or

4 nk_1 $(m = 0)$

Proof. Let G be a graph with Eigen values $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ recall (4.6). That is, among the known lower bounds of λ_1 is the following $\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}}$ where $d_1, d_2, ...d_n$ the degree sequence of G. Then by Cauchy-schwartz inequality we have

$$\begin{aligned} \sum_{i=2}^{n} |\lambda_i| &\leq \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i} \\ &= \sqrt{(n-1)\left(\sum_{i=1}^{n}(\lambda_i^2 - \lambda_1^2)\right)} \end{aligned}$$

Then since $\sum \lambda_i^2 = 2m = traceA^2$, we have

$$\sum_{i=^2}^{n} |\lambda_i| \leq \sqrt{(n-1)(2m - \lambda_1^2)}$$

Since $\lambda_1 > \lambda_i$ for all i and $\sum_{i=1}^{n} \lambda_i = 0, \lambda_i$ must be non negative, and hence $\lambda_1 = |\lambda_1|$ Therefore

$$\begin{aligned} E(G) &= \sum_{i=1}^{n} |\lambda_i| \\ &= \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \\ &= \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} \end{aligned} \tag{4.8}$$

That is,

$$E(G) \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} \tag{4.9}$$

Let $F(X) = x + \sqrt{(n-1)(2m - x^2)}$, then note that the function $F(x)$ decreases for $\sqrt{\frac{2m}{n}} \leq x \leq \sqrt{2m}$ and from (4.6) we will get that,

$$\sqrt{\frac{2m}{n}} \leq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} \leq \lambda_1$$

Therefore we can see that $F(\lambda_1) \leq F\left(\sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}\right)$

That is,

$$\lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)} \leq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} d_i^2}{n}\right)}$$

Now by (4.9) it is obvious that

$$E(G) \leq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} d_i^2}{n}\right)} \tag{4.10}$$

Now if G is $\frac{n}{2}K_2$ then we have $m = \frac{n}{2}$ and $d_1 = d_2 = ... = d_n = 1$

Thus

$$\begin{aligned} RHS\ of\ (4.10) &= \sqrt{\frac{\sum_{i=1}^{n} 1^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} 1^2}{n}\right)} \\ &= 1 + \sqrt{(n-1)(n-1)} \\ &= 1 + n - 1 = n \end{aligned}$$

Also

$$\begin{aligned} E(\frac{n}{2}K_2) &= \frac{n}{2}E(K_2) \\ &= \frac{n}{2}2(2-1) \qquad since\ E(Kn) = 2(n-1) \\ &= n \end{aligned}$$

i.e, the equality in (4.10) holds for $G = \frac{n}{2}K_2$.

Now let $G = K_n$ then $m = \frac{n(n-1)}{2}$, the degree sequence $d_1 = d_2 = ... = d_n = n-1$,

$$\begin{aligned} LHS\ of\ (4.10) &= \sqrt{\frac{\sum_{i=1}^{n}(n-1)^2}{n}} + \sqrt{(n-1)\left(\frac{2n(n-1)}{2} - \frac{\sum_{i=1}^{n}(n-1)^2}{n}\right)} \\ &= (n-1) + (n-1)\sqrt{n-(n-1)} \\ &= 2(n-1) \end{aligned}$$

Thus here also holds the equality in 4.10.

Now if $G = nK_1$, that is $m = 0$ then $d_1 = d_2 = \ldots = d_n = 0$. Since here G is the totally disconnected graph, $E(G) = 0$, also LHS of (4.10)$= 0 + \sqrt{(n-1)(0-0)} =$ 0 therefore here also the equality of (4.10) holds. Similarly we can prove that this equality for non-complete connected strongly regular graph with two non trivial Eigen values both having absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{(n-1)}}$

Conversely if

$$E(G) \leq \sqrt{\frac{\sum_{i=1} d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_i d_i^2}{n}\right)}$$

then by above argument we see that

$$\lambda_1 = \sqrt{\frac{\sum_i d_i^2}{n}} = \sqrt{\frac{\sum_i k^2}{n}} = k = \frac{2m}{n}.$$

it follows that G is a regular graph or a semi regular graph and $m > 0$ then $m = \frac{nk}{2}$ and $d_i = k$ for all $i = 1, 2, \ldots, n$
Therefore $\lambda_1 = \sqrt{\frac{\sum_i d_i^2}{n}} = \sqrt{\frac{\sum_i k^2}{n}} = k = \frac{2m}{n}$ $\{$ by a result from the paper [8] by J. H. Koolen and V. Moulton$\}$. Now,since equality must also hold in the cauchy schwartz inequality given above, we have $|\lambda_i| = \sqrt{\frac{2m-(\frac{2m}{n})^2}{(n-1)}}$,for $2 \leq i \leq n$. Hence we are reduced to three possibilities:either G has two eigenvalues with equal absolute values, in which case G must equal $(\frac{n}{2})K_2$, or G has two eigenvalues with distinct absolute values,in which case G must equal k_n, or G has three eigenvalues with distinct absolute values equal to $\frac{2m}{n}$ or $\sqrt{\frac{2m-(\frac{2m}{n})^2}{(n-1)}}$, in which case G must be a non-complete connected strongly regular graph [4]. This completes the proof. $\square$

Remark 4.3.1. Note that $\sqrt{\frac{\sum d_i^2}{n}} \geq \frac{2m}{n}$. Thus since $\sum_{i=1}^{n} d_i^2 = 2m$, we have $4m^2 = (\sum_{i=1}^{n} d_i)^2$ and since $F(x) = x + \sqrt{(n-1)(2m - x^2)}$

decreases for $\sqrt{\frac{2m}{n}} \leq x < \sqrt{2m}$. We have

$$E(G) \leq F\left(\sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}\right) \leq F\left(\frac{2m}{n}\right)$$

But since $F(\frac{2m}{n}) = \frac{2m}{n} + \sqrt{(n-1)(2m - \frac{4m^2}{n^2})}$ which is the inequality (4.5), given in the beginning of this section.

Applications

The concept of graph energy is widely used in chemistry where certain numerical quantities, such as the heart of formation of hydrocarbon, are related to the total $\pi-$ electron energy that can be calculated as the energy of an appropriate "molecular" graph. That is the concept of Graph energy is used to approximate the total π electron energy molecules. Very recently graph energy has become a quantity of interest to mathematicians, and several have been introduced.

There is no reason that one cannot study this quantity for an arbitrary graph, and so Gutman defines the energy of a graph to be sum of the absolute values of its Eigen values. Formulate and bound for this expression are useful for theoretical chemists, for whom this value can take on physical significance. For mathematicians, the concept leads to many interesting problems which are not necessarily identical to determining the spectrum of a graph.

Conclusion

The energy of a graph E(G) is the sum of absolute values of its Eigen values. As the sum of the absolute values of Eigen values, E(G) is always greater than or equals to zero and energy of the totally disconnected graph is 0. The complete graph K n has energy $2(n-1)$. We have shown that the energy of a disconnected graph is the sum of the energies of its connected components. For a simple graph G with n vertices and m edges $E(G) \leq \sqrt{2mn(n-1)}$

Also we deals with hyper-energetic and non hyper energetic graphs and examples of non hyper-energetic graphs and all subdivision graphs are non hyper-energetic. At that last chapter we discovered some bounds for graph energy. If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, ..., d_n$ then,

$$E(G) \leq \sqrt{\frac{\sum_i d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_i d_i^2}{n}\right)}$$

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