**Project Report** 

# On

# SPECTRAL GRAPH THEORY: PROPERTIES AND APPLICATIONS

Submitted

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in

MATHEMATICS

by

# HARIPRIYA H

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Under the Supervision of

NISHA OOMMEN



DEPARTMENT OF MATHEMATICS ST. TERESA'S COLLEGE (AUTONOMOUS) ERNAKULAM, KOCHI - 682011 APRIL 2022

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# CERTIFICATE

This is to certify that the dissertation entitled, SPECTRAL GRAPH THE-ORY : PROPERTIES AND APPLICATIONS is a bonafide record of the work done by Ms. HARIPRIYA H under my guidance as partial fulfillment of the award of the degree of Master of Science in Mathematics at St. Teresa's College (Autonomous), Ernakulam affiliated to Mahatma Gandhi University, Kottayam. No part of this work has been submitted for any other degree elsewhere.

Date: 26.5.2022 Place: Ernakulam

NISHA OOMMEN Assistant Professor, Department of Mathematics, St. Teresa's College(Autonomous), Ernakulam.

1: DIV.Y.D. MARY. DAISES



Dr.Ursala Paul Assistant Professor and HOD Department of Mathematics, St. Teresa's College(Autonomous), Ernakulam.

2: MARY. BUNDA.

External Examiners



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# DECLARATION

I hereby declare that the work presented in this project is based on the original work done by me under the guidance of **NISHA OOMMEN**, Assistant Professor, Department of Mathematics, St. Teresa's College(Autonomous), Ernakulam and has not been included in any other project submitted previously for the award of any degree.

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Date: 26.5.2022

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HARIPRIYA H

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HARIPRIYA H SM20MAT004

Date: 26.5.2022



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# Chapter 1

# INTRODUCTION AND HISTORICAL OUTLINE

## 1.1 INTRODUCTION

Spectral graph theory is a branch of mathematics that studies graphs by using spectral properties of a graph and its associated matrices.

Spectral graph theory is the study of properties of a graph in relation to the characteristic polynomial, Eigenvalues and eigenvector's of matrices associated with the graph, such as its adjacency matrix or laplacian matrix. The adjacency matrix of an undirected graph is a real symmetric matrix and it is orthogonally diagonalize. Also its eigenvalues are real algebraic integers. It also depends upon the vertex labelling and its spectrum is graph invariant. L. Collatz and U. Sinogowitz first began the exploration of this topic in 1957. Originally spectral graph theory analyses adjacency matrix of a graph, especially its eigenvalues. Central goal of graph theory is to deduce the main properties and structure of a graph from its invariant. The eigenvalues are strongly connected to almost all key invariant of a graph. They hold a wealth of information about graphs. This is what spectral graph theory concentrates on.

There are numerous applications of mathematics specifically spectral graph theory with in science and many other fields. This paper is an exploration of recent application of spectral graph theory. The main focus is on the characteristic polynomial and eigenvalues that it produces. Because most of the applications involve specific eigenvalues. For example in chemistry non saturated hydrocarbons are represented by graphs. The energy level of electrons in such molecules are the eigenvalues of corresponding graph. The stability of the molecule as well as other chemically relevant facts are closely connected with graph spectrum and their eigenvalues

## 1.2 HISTORY

In mathematics origin of graph theory can be traced to 1735, when the Swiss mathematician **Leonardo Euler** solved the Kornberg bridge problem. graph theory is a study of graphs which are mathematical structures used to model pairwise relations between objects. Graph theory is also important in life.

Spectral graph theory is a branch of mathematics. Spectral graph theory emerged in 1950s and 1960s. It is a relationship between structural and spectral properties of a graphs. Besides graph theoretic research on the relationship between structural and spectral properties of graph, another major source was research in quantum chemistry, the 1980 monograph spectra of graph by **Doob and Sachs** summarised nearly all research to date in the area. In 1988 it was updated by Recent results in the theory of graph spectra. The 3rd edition of spectra of graph contains summary of the contributions to the subject

Dis create geometric analysis created and developed by **Toshikazu Sunanda** in the 2000s deals with spectral graph theory in terms of dis create laplacian associated with graphs and find applications in various field. In most recent years spectral graph theory has expanded to vertex varying graphs often encountered in many real- life applications.

# Chapter 2

# PRELIMINARIES

### 2.1 GRAPHS

A graph G is a finite non empty set of points called vertices and together with a set of ordered pair of distinct vertices called edges. the set of edges may be empty. The degree of a vertex is the no of edges incident on it. A graph is regular all vertices have equal degree and complete each pair of vertices joined by an edge. Two vertices are adjacent there is an edge connecting them. The cardinality of vertex set is called order of G. The cardinality of edge set is called size of G. A walk  $V_iV_j$  is a finite sequence of adjacent vertices that begins at vertex  $V_i$  and ends at vertex  $V_j$ .

A simple graph is an undirected graph in which no parallel edges and no loops. An undirected graph whose edges are not directed.

A directed graph is a graph in which the edges are directed by arrows.

Two vertices are joined by more than one edge becomes a **multi graph**. When a pair of vertices is not distinct then there is a self-loop. A graph admits multiple edges and loops is called a **Pseudo-graph**.

Graphs G and H are said to be **Isomorphic graph** G, If there is a vertex bijection  $f: V(G) \to V(H)$ . such that for all u,v belongs to V(G). u and v are adjacent in G if and only if F(u)

and F(v) are adjacent in H.

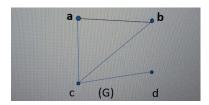
#### 2.2 SOME GRAPH THEORETIC DEFINITIONS

There are a great deal of importance and applications in representing a graph G in its matrix form. One of the key ways to do this is through the adjacency matrix A. The rows and columns of adjacency matrix represent the vertices and the elements tell whether there is an edge between any two vertices. Given an element  $a_{ij}$ 

$$a_{ij} = \begin{cases} 1 & ifa_i \text{ and } a_j \text{ are connected} \\ 0 & otherwise. \end{cases}$$
(2.1)

#### Adjacency matrix:

Let G be a graph. The adjacency matrix G denoted by A(G) whose rows and columns are indexed by the vertices where u v entry is equal to the number of edges between u and v. A(G) is a real symmetric matrix whose diagonal entries are equal to zero. **Example** of adjacency matrix is given below,



Adjacency matrix of above graph is given by

 $\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ 

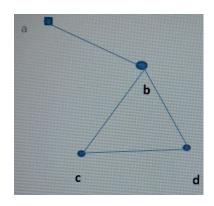
Note that the diagonal of an adjacency matrix of a graph contains only zeros because there is no self-loops. Our graph has no multiple edges or loops. This cause the trace of adjacency matrix, written by tr(A), the sum of its main diagonal, to be zero. Also when A represent a graph, it is square, symmetric and all of the elements are non negative.

#### The Laplacian:

The Laplacian is an alternative approach to the adjacency matrix. Laplacian L of a graph is the square matrix that correspond to the vertices of a graph. The main diagonal of the matrix represents the degree of the vertices.

$$A_{ij} = \begin{cases} -1 & ifv_i \text{ and } v_j \text{ are adjacent} \\ 0 & otherwise. \end{cases}$$
(2.2)

Laplacian also derived from D-A where D is the diagonal matrix whose entries represent the degree of the vertices and A is the adjacency matrix. **Example** of a laplacian matrix is given below



$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}.$$

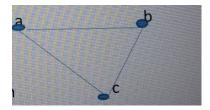
**Characteristic polynomial**: The characteristic polynomial of a graph of order n is the determinant of  $(\lambda I - A)$ ,

where I is a n n x n identity matrix.

The general form of a characteristic polynomial is

$$\lambda^n + C_1 \lambda^{n-1} + \dots + C_n \lambda^n \tag{2.3}$$

**Example** Consider the matrix given below:



$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$
$$\det(\lambda I - A) =$$

$$det \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} - \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = det \begin{pmatrix} \lambda & -1 & -1 \\ -1 & \lambda & -1 \\ -1 & -1 & \lambda \end{pmatrix} = \lambda^3 - 3\lambda^2 - 2 \quad (2.4)$$

The coefficients of the characteristic polynomial is that coincide with the matrix A of a graph G has following characteristic

- $c_1 = 0$
- $-c_2$  is the number of edges of G
- $-c_3$  is twice the number of triangles in G

The characteristic polynomial is enormously important in spectral graph theory. Because it is an algebraic construction that contain graphical information. It will be more explored in chapter3.

The root of a characteristic polynomial is **eigenvalues**. From the above example the characteristic polynomial

$$\lambda^3 - 3\lambda^2 - 2 \tag{2.5}$$

equal to zero and solving gives the eigenvalue -1,-1,2.

Eigenvalues are the heart of understanding the properties and structure of graph. **Connected**: A graph is connected if for every pair of vertices u and v ,there is a walk from u to v.

A tree is a connected graph that has no cycles.

A spanning tree of a graph is a spanning sub graph that is a tree.

The complexity of G denoted by k(G), is the number of spanning trees of G.

#### Bipartite graphs-

A **bipartite graph** G is one whose vertex set V can be partitioned into two subset U and W such that each edge of G has one end point in U and one in W . the pair U,W is called bi partition of G and U and W are called bi partition subset .

The spectrum of a bipartite graph is symmetric around 0.

**Theorem**: If G is a bipartite graph  $\lambda$  is an eigenvalue and  $-\lambda$  is also an eigenvalue

**Proof**: let G be a bipartite graph.  $U = u_1 u_2 \dots u_n$  and  $W = w_1 w_2 \dots w_n$ . where u and w are partite set of V(G). then all edges are of the form  $u_i w_j$  where  $u_i$  belongs to U and  $w_j$  belongs to W. also no edges go from  $u_i$  to  $u_j$  or  $w_i$  to  $w_j$ . This makes the adjacency matrix of G

$$\mathbf{A} = \begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix}.$$

where B is an n by m matrix.because  $\lambda$  is an eigenvalue.we know  $Av = \lambda v$ .so

$$\begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$$
(2.6)

using simple matrix multiplication  $By = \lambda x$ .

Multiplying both sides by negative one we get  $B(-y) = -\lambda x$ . The second equation that results from the matrix multiplication is  $B^t x = \lambda$  y and  $\lambda y = -\lambda - y$ .  $B^t x = -\lambda - y$ . This gives the matrix equation

$$\begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = -\lambda \begin{pmatrix} x \\ y \end{pmatrix}$$
(2.7)

giving us the eigenvalue  $-\lambda$ .

**Corollary**: The spectrum of a bipartite graph is symmetric around zero.

**Complete graph** : A complete is one in which every pair of vertices is joined by an edge. The complete graph  $k_p$  is determined by its spectrum.

**Eigenvalues of graph**: For a matrix A in  $\mathbb{R}^{n*n}$ , a number  $\lambda$  is an eigenvalue if for some vector x not equal to zero  $Ax = \lambda x$ . The vector x is called an eigenvectors corresponding to  $\lambda$ . The sum of all eigenvalues if a graph is always zero.

# 2.3 ALGEBRAIC MULTIPLICITY AND GEOMETRIC MULTIPLICITY:

Algebraic multiplicity of an eigenvalue is the no of times that the value occurs as a root of characteristic polynomial.

**Geometric multiplicity** is the dimension of eigen space or subspace spanned by all of its eigenvectors.

**Theorem**: If a matrix is real symmetric, each eigenvalue of the graph relating to the matrix is real.

**Proof**: The proof follows from spectral theorem from linear algebra. A be a real symmetric matrix. There exist an orthogonal matrix Q such that  $A = QAQ^{-1} = QAQ^{T}$ , where A is a real diagonal matrix, the eigenvalue of A appear on the diagonal of A, while the columns of Q are the corresponding eigenvectors. The entries of an adjacency matrix are real and adjacency symmetric. Therefore, all the eigenvalues of an adjacency matrix are real.

The geometric and algebraic multiplicity of each eigenvalue of a real symmetric matrix is equal.

If a graph is connected the largest eigenvalue has multiplicity of one.

# Chapter 3

# SPECTRAL GRAPH THEORY

## 3.1 SPECTRAL GRAPH

**spectral graph theory** is the study of properties of a graph in relation to the characteristic polynomial, eigenvalues and eigen vectors of a matrices associated with the graph. Main matrix used in this theory is adjacency or Laplacian matrix.

Co spectral graph: The construction of co spectral graphs has been prominent in the theory of graph spectra. There are two methods of constructing the co spectral graphs. One method is a kind of 'cut and paste': a piece of graphs is excised and replaced by a new piece in such a way that the spectrum is unchanged, but the new graph is not isomorphic to old one. Second method is 'product method'. Products of graphs are taken.

Two graphs are called co spectral they have same spectrum.co spectral graphs need not be isomorphic, but isomorphic graphs are always co spectral.

#### Examples

Almost all trees are co spectral.

A pair of regular graphs are co spectral if and only if their complements are co spectral.

A pair of distance regular graph are co spectral if and only if they have same intersection array.

Another important sources of co spectral graphs are the point col-linearity graphs

and line intersection graphs. These graphs are always co spectral but non isomorphic.

## 3.2 SPECTRUM OF A GRAPH

The spectrum of a real symmetric matrix is the list of its eigenvalues, where each eigenvalue with multiplicity k appears k times in the list. If matrix is n x n then its spectrum has length n.

#### Definition

The **spectrum** of a graph G is a set of eigenvalues of G together with their algebraic multiplicities or the number of times that they occur".

#### Graphs determined by their spectrum:

A graph G is said to be determined by their spectrum if any other graph with the same spectrum as G is isomorphic to G.

Some examples of a families of graphs that are determined by their spectrum include:

- The complete graph
- The finite star like trees

if a graph has k distinct eigenvalues  $\lambda_1 > \lambda_2 > \dots > \lambda_k$  with multiplicities  $m(\lambda_1) \dots m(\lambda_k)$ . Then the spectrum of G can be written as

 $\operatorname{spec}(G) =$ 

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \dots & \lambda_k \\ m(\lambda_1) & m(\lambda_2) & \dots & m(\lambda_k) \end{pmatrix}.$$

#### Example of a spectrum of a graph



corresponding matrix of above figure is given below

 $\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$ 

The characteristic polynomial is  $4\lambda^4 - 4\lambda^2$ 

with eigenvalues 0 0 2 -2. Our graph has 3 distinct eigenvalues -2,0 and 2. Hence the spectrum of the graph G is

$$\operatorname{spec}(G) =$$

$$\begin{pmatrix} -2 & 0 & 2 \\ 1 & 2 & 1 \end{pmatrix}$$

One consistent question in graph theory is when is a graph characterised by its spectrum? Properties that cannot be determined by spectrally can be determined by compare two non isomorphic graphs with the same spectrum.

It is clear that two graphs are structurally different with different adjacency matrices and they have same spectrum.

# 3.3 SPECTRAL CHARACTERIZATIONS OF CERTAIN GRAPHS

Given the spectrum or some spectral characteristic of a graph, determine all graph from a given class of graphs having the given spectrum, or the given spectral characteristics.

In this sections describe some cases in which graphs are characterized by their spectra. All graphs in this section is finite un directed and simple.

#### Definition

We say that a graph is characterized by its spectrum if the only graphs are co spectral with G and isomorphic to G. Examples include complete graphs and graph with one edge.

Given spectrum of a graph G we can always establish whether or not G is reg-

ular.it follows that if G or G is regular of degree one then G is characterized by their spectrum.

**Remark**: Any regular graph of degree 2 is characterized by their spectrum.

for each positive integer n, the complete graph  $K_n$ , n is characterised by their spectrum.

**Spectrum of complete graph**: let us consider the complete graph  $K_n$  on n vertices. Its adjacency matrix is A=J-I.

$$A = \begin{pmatrix} 0 & 1 & 1 \dots 1 \\ 1 & 0 & 1 \dots 1 \\ \dots \\ 1 & 1 & 1 \dots 0 \end{pmatrix}$$

$$\lambda = w + w^{2} + \dots + w^{n-1}$$
(3.1)

$$\lambda_w = w + w^2 + \dots + w^{n-1} \tag{3.1}$$

n-1 if w=1-1 if  $w \neq 1$  $\operatorname{spec}(k_n) =$ 

$$\binom{n-1 \quad -1}{1 \quad n-1}.$$

**Spectrum of cycle**: let us consider the directed n cycle  $D_n$ . Eigenvectors are  $1, \lambda \dots \lambda^{n-1}$ , where  $\lambda^n = 1$  and the corresponding eigen value is  $\lambda$ . Thus the spectrum consist precisely the complex n roots of unity  $e^{2\Pi i j/n}$ .  $(j = 0, 1 \dots n-1)$ . Consider the undirected n cycle  $C_n$ . Then  $A = B + B^T$ . B is the adjacency matrix of  $C_n$  so that the spectrum consist the numbers  $2\cos(2\Pi j/n)$ .  $(j = 0, 1 \dots n - 1)$ . The graph is regular of valency 2. So the laplacian spectrum consist the numbers  $2 - 2\cos(2\Pi j/n).$ 

**Spectrum of the path**: Consider the undirected path  $P_n$ . The ordinary spectrum consist of the numbers  $2\cos(\Pi j/(n+1))$ . (j=0,1...n). the laplacian spectrum is  $2 - 2\cos(\Pi j/n) . (j = 0, 1 ... n - 1).$ 

### 3.4 THE LAPLACIAN

**The Laplacian**: The Laplacian is an alternative approach to the adjacency matrix. The Laplacian L of a graph is the square matrix that correspond to the vertices of a graph. The main diagonal of the matrix represents the degree of the vertices. LG = -1 if  $v_i$  and  $v_j$  are adjacent 0 otherwise. The Laplacian also derived from D-A where D is the diagonal matrix whose entries represent the degree of the vertices and A is the adjacency matrix.

**Theorem**: The smallest eigenvalue of L is zero.

**Proof**: This is a direct result from the Laplacian matrix being a positive semi definite matrix. It will have n real Laplacian eigenvalue  $0 = \lambda_1 \leq \lambda_2 \leq \ldots \lambda_m$  (**positive semi definite matrix** whose eigen values are non-negative).

#### \* Basic properties of Laplacian matrix

For a graph G = (V, E),  $L_G = \Sigma L_G(u, v)$ . The eigen values of Laplacian matrix are real by realising that the Laplacian matrix of a graph is symmetric and consist of all entries. Therefore,  $L_G$  is self-ad joint. By the following theorem all eigen values of  $L_G$  are real.

**Theorem**: The eigen values of a self ad joint matrix are real.

**Proof**: Suppose  $\lambda$  is an eigen value of a self-ad joint matrix L. V is nonzero vector of  $\lambda$ . Then  $\lambda$  norm  $V^2 = \lambda < v, v >$ 

 $\lambda \operatorname{norm} V^2 = \lambda < v, v >$   $< \lambda v, v >$   $= \langle Lv, v >$   $= \langle v, Lv >$   $= \langle v, \lambda v >$   $= \lambda \langle v, v >$   $= \lambda \operatorname{norm} V^2.$ Here  $v \neq 0.$ Norm  $v^2 \neq 0.$ This proves that  $\lambda$  is real.

**Remark**: For a graph G eigen value  $L_G$  is non negative. The Laplacian of  $K_n$  has eigen value zero with multiplicity 1 and eigen value n with multiplicity n-1.

When we have a k regular graph a graph whose vertices all have degree k then there is linear relationship between eigen values of laplacian and eigenvalues of adjacency matrix A. if  $\theta_1 \theta_2 \dots \theta_n$  are the eigen values of L and  $\lambda_1 \lambda_2 \dots \lambda_n$  are the eigen values of A. Then  $\theta_i = k - \lambda_i$  this is a result of a graph being a regular graph. Giving us the relationship L=k I-A between the laplacian and adjacency matrix. No such relationship exists between the eigenvalues of laplacian and adjacency matrix of a non-regular graph.

**Theorem**: The algebraic connectivity is positive if and only if the graph is connected.

**proof**: If  $\lambda_2 > 0$  and  $\lambda_1 = 0$  then G must be connected. Because the eigen values of Laplacian are zero  $0 = \lambda_1 \leq \lambda_2 \leq \ldots \lambda_m$ 

This is direct result from the above theorem . If G is connected, then zero is the smallest eigenvalue.  $\lambda_2$  must be greater than zero and therefore positive.

# Chapter 4

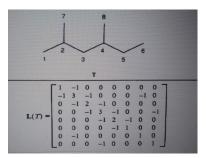
# APPLICATIONS OF SPECTRAL GRAPH THEORY

## 4.1 LAPLACIAN MATRIX AND ITS SPECTRUM

The Laplacian matrix, its spectrum and its polynomials are discussed in this section.

The Laplacian matrix L=L(G) of a simple graph G is defined as L = V - AA is the adjacency matrix and V is the degree of the matrix.

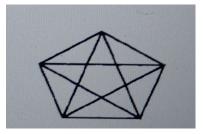
For example, Laplacian matrix of a tree T, depicting the carbon skeleton of 2,4 Di-methyl hexane is given below



The Laplacian matrix is a real symmetric matrix. The diagonalization of the Laplacian matrix of a graph G with N vertices gives N real eigenvalues  $x_i = 1, 2...N$ . The set of eigenvalues is referred to as the spectrum of the laplacian matrix of G or Laplacian spectrum of G. The smallest member of the laplacian spectrum is  $x_1$  is always equal to zero. Conventionally, the laplacian eigenvalues

are given in increasing order.  $0 = x_1 \leq x_2 \leq \ldots x_N$  The Laplacian spectrum of the complete graph  $K_N$  shows the following pattern:  $[0, N, N, N \dots]$ .

Thus, we can immediately write down the Laplacian spectrum of the kuratowski graph  $k_5$  as



[0, 5, 5, 5, 5].

In case of regular graphs, the eigenvalues  $x_i(L)$  of the Laplacian matrix are related to eigenvalues  $x_i(A)$  of the corresponding adjacency matrix as follows  $X_i(L) = D - x_i(A)$ .

D is vertex degree in a regular graph.

The Laplacian spectrum has number of interesting properties. It can be used to compute number of spanning trees of a poly cyclic graph G and also to find the energy of a graph.

#### 4.2 SPANNING TREES

The number of spanning trees of a graph can be calculated by using the simple formula based on the matrix tree theorem. "Let i and j be the vertices of a graph G and  $L_{ij}$  be the sub matrix of the Laplacian matrix G obtain by deleting the row i and the column j. Then the absolute value of the determinant of  $L_{ij}$  is equal to the number of spanning trees t(G) of G.

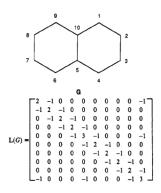
 $t(G) = det|(L_{ij})|$ 

$$t(G) = (1/N)\Pi xi$$

where t(G) is the no of spanning trees of G.

#### Example

1. consider a naphthalene graph G and the Laplacian matrix is given below



3. Using this method, we get eigenvalues of the Laplacian matrix. The set of eigenvalues is referred to as Laplacian spectrum.

Laplacian spectrum is [0.0000,0.3820,0.8851,1.3820,1.3820,2.6180,3.2541,3.6180,3.6180,4.8608]

4. Using this laplacian spectral values we can count the spanning trees of a graph given by the equation  $t(G) = (1/N)\Pi xi$ . Spanning trees of naphthalene graph is given by  $t(G) = (1/N)\Pi xi =$  $(1/10) [0.0000 \times 0.3820 \times 0.8851 \times 1.3820 \times 1.3820 \times 2.6180 \times 3.2541 \times 3.6180 \times 3.6180] = 35.$ 

## 4.3 ENERGY OF A GRAPH

The energy E(G) of a graph G is defined as follows

"G be a graph with n vertices and its spectrum consist the numbers  $\lambda_1, \lambda_2 \dots \lambda_n$ then  $E = E(G) = \Sigma |\gamma_i|$ 

L(G) denote the Laplacian energy of a graph G which is defined as sum of absolute values of the eigenvalues of a graph G,  $L(G) = \Sigma |\gamma_i|$  where  $\gamma_i$  be the eigenvalues of G."

5. From the above example energy of naphthalene graph G is  $E(G) = \Sigma$ 

[0.0000 + 0.3820 + 0.8851 + 1.3820 + 1.3820 + 2.6180 + 3.2541 + 3.6180 + 3.6180 + 4.8608] = 22.

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