

## Chapter 2

### Preliminaries

#### 2.1 Introduction

This chapter incorporates a number of definitions and results collected from standard textbooks and research publications on matrices, graphs, and semigraphs relevant to the works embodied in the subsequent chapters of the thesis. Mainly, the classic book on graph theory by F. Harary [17] has been consulted freely because, in spite of exponential growth in the number of publications of good books with every passing year, Harary seems unmatched even today. D. B. West [12], G. Chartrand and L. Lesniak [18] are also a few names consulted here and there. The very topic of the thesis viz. semigraph a generalization of the graph, being comparatively of recent origin, the bulk of the concepts, terminology and notations on it had to be borrowed from its originator E. Sampathkumar [15, 16]. Following Harary, the concept graph is used here to mean simple graphs only, i.e., graphs in which multigraphs and loops are prohibited. After recalling some matrix preliminaries in this chapter, the next few chapters outline the basic properties of some matrices associated with semigraph.

#### 2.2 Matrices [31, 44]

In this section, we review certain basic concepts on matrices for real entries. Relevant concepts and results are given omitting their proofs.

##### **Basic definitions:**

An  $m \times n$  matrix consists of  $mn$  real numbers arranged in  $m$  rows and  $n$  columns. The entry in  $i^{\text{th}}$  row and  $j^{\text{th}}$  column of the matrix  $A$  is denoted by  $a_{ij}$ . 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  $m = n$ .

Operations of matrix addition, scalar multiplication and matrix multiplication are basic and will not be recalled here. The transpose of the  $m \times n$  matrix  $A$  is denoted by  $A^T$  of order  $n \times m$  obtain by interchanging rows and columns of  $A$ .

A diagonal matrix is a square matrix  $A$  such that  $a_{ij} = 0, i \neq j$ . We denoted the diagonal matrix by  $A = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$ . When  $\lambda_i = 1$  for all  $i$ , this reduces to the identity matrix of order  $n$ , which we denote by  $I_n$  or often simply by  $I$ . The matrix  $A$  is upper triangular or lower triangular according as  $a_{ij} = 0, i > j$  or  $i < j$ . The transpose of an upper triangular matrix is lower triangular.

### **Trace and determinant:**

Let  $A$  be a square matrix of order  $n$ . The entries  $a_{11}, a_{22}, \dots, a_{nn}$  are said to constitute the (main) diagonal of  $A$ . The *trace* of  $A$  is defined as

$$\text{trace } A = a_{11} + a_{22} + \dots + a_{nn}.$$

It follows from this definition that if  $A$  and  $B$  are matrices such that both  $AB$  and  $BA$  are defined, then

$$\text{trace } AB = \text{trace } BA$$

The determinant of an  $n \times n$  matrix  $A$ , denoted by  $\det A$ , is defined as

$$\det A = \sum_{\sigma} \text{sgn}(\sigma) a_{1\sigma(1)} \dots a_{n\sigma(n)},$$

where the summation is over all permutations  $\sigma(1), \sigma(2), \dots, \sigma(n)$  of  $1, 2, \dots, n$ , and  $\text{sgn}(\sigma)$  is 1 or  $-1$  according as  $\sigma$  is even or odd.

### **Nonsingular matrices:**

A matrix  $A$  of order  $n \times n$  is said to be nonsingular if  $\text{rank } A = n$ ; otherwise the matrix is singular. If  $A$  is nonsingular, then there is a unique  $n \times n$  matrix  $A^{-1}$ , called the inverse of  $A$ , such that  $AA^{-1} = A^{-1}A = I$ . A matrix is nonsingular if and only if  $\det A$  is nonzero.

The cofactor of  $a_{ij}$  is defined as  $(-1)^{i+j} \det A(i|j)$ . The adjoint of  $A$  is the  $n \times n$  matrix whose  $(i, j)^{\text{th}}$  entry is the cofactor of  $a_{ji}$ . We recall that if  $A$  is nonsingular, then  $A^{-1}$  is given by  $\frac{1}{\det A}$  times the adjoint of  $A$ .

## Orthogonality:

Vector  $x, y$  in  $R^n$  are said to be orthogonal, or perpendicular, if  $x'y = 0$ . A set of vectors  $\{x_1, x_2, \dots, x_m\}$  in  $R^n$  is said to form an orthonormal basis for the vector space  $S$  if the set is a basis for  $S$ , and furthermore  $x_i x_j$  is 0 if  $i \neq j$ , and 1 if  $i = j$ . The  $n \times n$  matrix  $P$  is said to be orthogonal if  $PP^T = P^T P = I$ . It is also verified that if  $P$  is orthogonal then  $P^T$  is orthogonal.

## Eigenvalue and singular value decomposition of matrices:

An eigenvalue and eigenvector of a square matrix  $A$  are a scalar  $\lambda$  and a nonzero vector  $x$  so that

$$Ax = \lambda x.$$

Thus eigenvalue-eigenvector equation for a square matrix can be written as

$$(A - \lambda I)x = 0, \quad x \neq 0.$$

This implies that  $A - \lambda I$  is singular and hence  $\det(A - \lambda I) = 0$ .

A singular value and pair of singular vectors of a square or rectangular matrix  $A$  are a nonnegative scalar  $\sigma$  and two nonzero vectors  $u$  and  $v$  so that

$$Au = \sigma u$$

$$A^H v = \sigma v$$

The superscript on  $A^H$  stands for Hermitian transpose and denotes the complex conjugate transpose of a complex matrix.

If the matrix is real, then  $A^H = A^T$ .

The singular values and singular vector equations for a matrix are

$$AV = U\Sigma$$

$$A^H U = V\Sigma^H$$

Here  $\Sigma$  is a matrix the same size as  $A$  that is zero except possibly on its main diagonal. It turns out that singular vectors can always be chosen to be perpendicular to each other, so the matrices  $U$  and  $V$ , whose columns are the normalized singular vectors, satisfy  $U^H U = I$  and  $V^H V = I$ . In other words,  $U$  and  $V$  are orthogonal if they are real, or unitary if they are complex. Consequently,

$$A = U\Sigma V^H$$

with diagonal  $\Sigma$  and orthogonal or unitary  $U$  and  $V$ . This is known as the singular value decomposition (*SVD*) of a matrix  $A$ .

### **Characteristic polynomial:**

Let  $A$  be a  $n \times n$  matrix. The determinant  $\det(A - \lambda I)$  is a polynomial in the (complex) variable  $\lambda$  of degree  $n$  and is called the characteristic polynomial of  $A$ . The equation  $\det(A - \lambda I) = 0$

is called the characteristic equation of  $A$ . By the fundamental theorem of algebra, the equation has  $n$  complex roots and these roots are called the eigenvalues of  $A$ .

The eigenvalues might not all be distinct. The number of times an eigenvalue occurs as a root of the characteristic equation is called the algebraic multiplicity of the eigenvalue.

If we may factor the characteristic polynomial as

$$\det(A - \lambda I) = (\lambda_1 - \lambda)(\lambda_2 - \lambda) \dots (\lambda_n - \lambda).$$

The geometric multiplicity of the eigenvalue  $\lambda$  of  $A$  is defined to be the dimension of the null space of  $A - \lambda I$ . The geometric multiplicity of an eigenvalue does not exceed its algebraic multiplicity.

### **Spectral theorem:**

A square matrix  $A$  is called symmetric if  $A = A^T$ . The eigenvalues of a symmetric matrix are real. Furthermore, if  $A$  is a symmetric  $n \times n$  matrix, then according to the spectral theorem there exists an orthogonal matrix  $P$  such that

$$\begin{pmatrix} \lambda_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \lambda_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \lambda_n \end{pmatrix}$$

In the case of a symmetric matrix the algebraic and the geometric multiplicities of any eigenvalues coincide. Also, the rank of the matrix equals the number of nonzero eigenvalues, counting multiplicities.

## Diagonalizing matrices:

When  $v_1, v_2, \dots, v_r$  are eigenvector associated with distinct eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_r$  the set  $\{v_1, v_2, \dots, v_r\}$  is linearly independent. Eigenvectors associated with the same eigenvalue  $\lambda$  may be linearly dependent or independent. If we can find a basis of eigenvectors, and if  $P$  is the matrix with these eigenvectors as columns, then  $P^{-1}AP$  is a diagonal matrix. Conversely, if  $A$  is any square matrix and if we can find a matrix  $P$  for which  $P^{-1}AP$  is a diagonal matrix, then there is a basis of eigenvectors, and these eigenvectors form the columns of  $P$ ; in this case, we say that  $A$  is diagonalizable.

Every symmetric matrix  $A$  has an orthonormal basis of eigenvectors, and so is diagonalizable. Moreover, the corresponding transition matrix  $P$  is then an orthogonal matrix ( $P^T = P^{-1}$ ), the matrix  $P^TAP$  is diagonal, and the matrix  $A$  is called orthogonally diagonalizable.

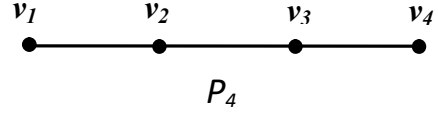
## 2.3 Graphs and its energy

Graph energy was first introduced by Serbian chemist and mathematician Ivan Gutman [22] in 1978 to approximate the total  $\pi$ -electron energy of a conjugate hydrocarbon as calculated by the Huckel molecular orbital (HMO) [21] method in quantum chemistry. In chemical literature graphs are used to represent different chemical objects like molecules, reactions etc. It depicted a chemical system whose vertices are atoms, electrons, molecules, groups of atoms etc. and edges are bound between molecules, bounded and non-bonded interactions, elementary reaction steps etc. Molecular graphs are a special type of chemical graph in which vertices are considered as individual atoms and edges as chemical bonds between them. Recall some definitions relevant to the present work as follows.

**Definition 2.3.1 [22] Energy of a graph:** If  $G$  is a simple connected graph of order  $p$  and size  $q$ . The adjacency matrix of  $G$  is the square matrix  $A = [a_{ij}]$  of order  $p$  whose entries  $a_{ij}$  are given by  $a_{ij} = 1$  if  $v_i$  and  $v_j$  are adjacent,  $a_{ij} = 0$  otherwise. The eigenvalues of  $A$  are the eigenvalues of  $G$ . The energy  $E(G)$  of a graph  $G$  is the sum of the absolute values of the eigenvalues of  $A$ .

**Example 2.3.1** Consider the path  $P_4$  as depicted in **Figure 2.1**, then its adjacency matrix is given by

$$A(P_4) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



**Figure 2.1**

The eigenvalues of  $A(P_4)$ , are  $-1.618034, 1.61803, -0.618034$  and  $0.618034$

Thus,

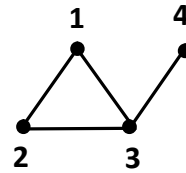
$$\begin{aligned} E(P_4) &= \sum_{i=1}^4 |\lambda_i| \\ &= |-1.618034| + |1.618034| + |-0.618034| + |0.618034| \\ &= 4.472136 \end{aligned}$$

Therefore, the energy of  $P_4$  is 4.472136.

**Definition 2.3.2 [19] Distance energy of a graph:** If  $G$  be a connected graph with  $p$  vertices and  $q$  edges, the distance matrix or  $D$ -matrix  $D = [d_{ij}]$ , is a square matrix of order  $p$  where,  $d_{ij}$  is the distance between the two vertices  $v_i$  and  $v_j$ . The  $D$ -Matrix  $D(G)$  of  $G$  is symmetric, and all of its eigenvalues  $\mu_1, \mu_2, \mu_3, \dots, \mu_p$  are all real, form  $D$ -spectrum of  $G$ . Then, distance energy or  $D$ -energy is defined as the sum of the absolute values of its  $D$ -eigenvalues.

**Example 2.3.2** Consider the Graph  $G(V, X)$  as shown in the **Figure 2.2**, then Distance matrix of  $G$  is given by

$$A_D(G) = \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 1 & 2 \\ 1 & 1 & 0 & 1 \\ 2 & 2 & 1 & 0 \end{pmatrix}$$



**Figure 2.2**

The characteristic equation of  $A_D(G)$  is  $-\lambda^4 + 12\lambda^2 + 18\lambda + 7 = 0$ .

**Definition 2.3.3 [6] Color energy of a graph:** Let  $G$  be a vertex-colored graph of order  $n$ . Then the color matrix of  $G$  is the matrix  $A_c(G) = (a_{ij})_{n \times n}$  for which

$$\begin{aligned} a_{ij}(v_i, v_j) &= 1 && \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ &= -1 && \text{if } v_i \text{ and } v_j \text{ are non-adjacent with } c(v_i) = c(v_j), \\ &= 0, && \text{otherwise,} \end{aligned}$$

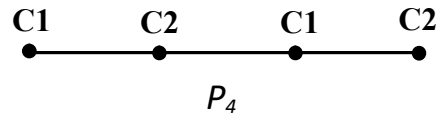
Where  $c(v_i)$  is the color of the vertex  $v_i$  in  $G$ . Recall that, the vertices of the graph  $G$  are colored so that two adjacent vertices always have different color.

The color energy of a graph  $G$  with respect to a given coloring is the sum of the absolute values of eigenvalues of the color matrix  $A_c(G)$ .

**Example 2.3.3** Consider the path  $P_4$  as shown in **Figure 2.3**, which is a bipartite graph and so, its chromatic number  $\chi(P_4) = 2$ .

The color matrix of  $P_4$  is given by

$$A_c(P_4) = \begin{pmatrix} 0 & 1 & -1 & 0 \\ 1 & 0 & 1 & -1 \\ -1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{pmatrix}$$



**Figure 2.3**

Then eigenvalues of  $A_c(P_4)$ , are -2.5615528, 1.5615528, 1 and 0. Therefore, the color energy of  $P_4$  with minimum number of colors is 5.1231056.

**Definition 2.3.4 [5] Minimum covering energy of a graph:** Suppose  $G(V, X)$  be a graph of order  $n$  and size  $m$ , with vertex set  $V$  and edges set  $X$ . Let  $C$  subset of  $V$  be the minimum covering set of a graph  $G$ . The minimum covering matrix of  $G$  is the square matrix  $A_{mc}(G) = (a_{ij})$  of order  $n$ , where

$$\begin{aligned} a_{ij} &= 1 && \text{if } v_i v_j \in E \\ &= 1 && \text{if } i = j \text{ and } v_i \in C \\ &= 0 && \text{otherwise.} \end{aligned}$$

And the minimum covering energy of the graph  $G$  is defined as  $E_{mc}(G) = \sum_{i=1}^n |\lambda_i|$  where  $\lambda_1, \lambda_2, \dots, \lambda_n$  are eigenvalues of the minimum covering matrix  $A_{mc}(G)$ .

**Example 2.3.4** Consider the path  $P_4$  as depicted in the **Figure 2.1**, and let its minimum covering set be  $C = \{v_1, v_3\}$  then

its adjacency matrix is given by

$$A_{mc}(P_4) = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Characteristic equation of  $A_{mc}(P_4)$  is  $\lambda^4 - 2\lambda^3 - 2\lambda^2 + 3\lambda + 1 = 0$ .

The minimum covering eigenvalues are

$$\frac{(1-\sqrt{7+2\sqrt{5}})}{2}, \quad \frac{(1+\sqrt{7+2\sqrt{5}})}{2}, \quad \frac{(1-\sqrt{7-2\sqrt{5}})}{2}, \quad \frac{(1+\sqrt{7-2\sqrt{5}})}{2}$$

and therefore, the minimum covering energy is

$$E_{mc}(P_4) = \sqrt{7 + 2\sqrt{5}} + \sqrt{7 - 2\sqrt{5}}.$$

**Definition 2.3.5 [29] Minimum covering distance energy:** Suppose  $G(V, X)$  be a graph of order  $n$  and size  $m$ . Let  $C$  be a subset of the vertex set  $V$ , is the minimum covering set of a graph  $G$ . The minimum covering distance matrix of  $G$  is the square matrix of order  $n$  defined as  $A_{MD}(G) = [d_{ij}]$ ,

where  $d_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } v_i \in C \\ d(v_i, v_j) & \text{otherwise.} \end{cases}$

The characteristic polynomial of  $A_{MD}(G)$  is denoted by  $P_n(G, \lambda) = \det[\lambda I - A_{MD}(G)]$ . The minimum covering eigenvalues of the graph  $G$  are the eigenvalues of  $A_{MD}(G)$ . Since  $A_{MD}(G)$  is real and symmetric, its eigenvalues are all real number and we label them in non-increasing order  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . The minimum covering distance energy of  $G$  is defined as  $E_{MD}(G) = \sum_{i=1}^n |\lambda_i|$ .

**Example 2.3.5** Consider the graph  $G$  as shown in **Figure 2.4**, then  $C = \{1, 2, 5\}$  is one of the minimum covering set for the graph  $G$ .



The minimum covering Distance matrix of  $G$  is given by

$$A_{MC}(G) = \begin{pmatrix} 1 & 1 & 2 & 1 & 1 & 2 \\ 1 & 1 & 1 & 2 & 1 & 2 \\ 2 & 1 & 0 & 2 & 1 & 2 \\ 1 & 2 & 2 & 0 & 1 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 1 & 0 \end{pmatrix}$$

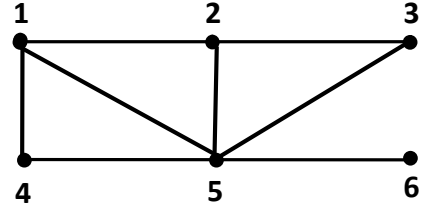


Figure 2.4

Characteristic equation is  $\lambda^6 - 3\lambda^5 - 33\lambda^4 - 50\lambda^3 + 5\lambda^2 + 21\lambda - 5 = 0$

Minimum covering distance eigenvalues are approximately equal to  $-2.4142$ ,  $-2.2203$ ,  $-1$ ,  $0.2837$ ,  $0.4142$ ,  $7.9366$ .

Thus,

$$\begin{aligned} E_{MC}(G) &= \sum_{i=1}^6 |\lambda_i| \\ &\approx |-2.4142| + |-2.2203| + |-1| + |0.2837| + |0.4142| + |7.9366| \\ &\approx 14.2691 \end{aligned}$$

Therefore, the Minimum covering distance energy of  $G$  is 14.2691.

**Definition 2.3.6 [30] Minimum covering color energy of a graph:** Let  $G$  be a vertex-colored graph of order  $n$ . Let  $C$  subset of  $V$  be the minimum covering set of a graph  $G$ . Then the minimum covering color matrix of  $G$  is the matrix  $A_{mc}^c(G) = (a_{ij})_{n \times n}$  of which,

$$\begin{aligned} a_{ij}(v_i, v_j) &= 1 && \text{if } v_i \text{ and } v_j \text{ are adjacent or if } i = j \text{ and } v_i \in C \\ &= -1 && \text{if } v_i \text{ and } v_j \text{ are non-adjacent with } c(v_i) = c(v_j), \\ &= 0 && \text{otherwise.} \end{aligned}$$

where  $c(v_i)$  is the color of the vertex  $v_i$  in  $G$ . The minimum covering color energy  $E_{mc}^c$  of a graph  $G$  with respect to a given coloring is the sum of the absolute value of eigenvalues of the minimum covering color matrix  $A_{mc}^c(G)$ .

**Example 2.3.6** Consider the graph  $G$  with vertex set  $V = \{1, 2, 3, 4\}$  with the minimum colors  $C_1, C_2, C_3$  and  $C_2$  respectively as shown in **Figure 2.5**. And let  $C = \{1, 2\}$  be the minimum covering set for the graph  $G$ .

Then the minimum covering color matrix of  $G$  is given by

$$A_{mc}^c(P_4) = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$$

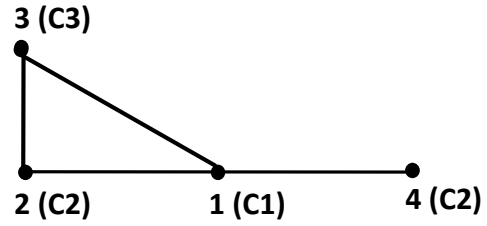


Figure 2.5

Characteristic equation is  $\lambda^4 - 2\lambda^3 - 4\lambda^2 + 4\lambda + 4 = 0$

Minimum covering color eigenvalues are approximately equal to 1.41421, -1.41421, 2.73205, -0.73205.

Therefore, the Minimum covering color energy of  $G$  is  $E_{mc}^c(G) \approx 6.29253$ .

## 2.4 Semigraphs:

**Definition 2.4.1 [15]** A semigraph is a pair  $G(V, X)$  where  $V$  is a non-empty set of elements called vertices and  $X$  is a set of  $n$ -tuples called edges of distinct vertices for various  $n \geq 2$  satisfying the conditions:

- i. Any two edges have at most one vertex in common.
- ii. Two edges  $E_1 = (u_1, u_2, \dots, u_p)$  and  $E_2 = (v_1, v_2, \dots, v_q)$  are considered to be equal if and only if  $p = q$  and either  $u_i = v_i$  or  $u_i = v_{p-i+1}$  for  $1 \leq i \leq p$ . In other words, the edge  $(u_1, u_2, \dots, u_{p-1}, u_p)$  is the same as the edge  $(u_p, u_{p-1}, \dots, u_2, u_1)$ .

In the edge  $E = (u_1, u_2, \dots, u_p)$  of a semigraph  $G = (V, X)$ , the vertices  $u_1$  and  $u_p$  are called the end vertices and all vertices in between  $u_1$  and  $u_p$  are called the middle vertices (m-vertices) of  $E$ . If any one of the vertices  $u_i$ ,  $2 \leq i \leq p-1$  is also an end vertex of another edge then this vertex is called the middle-end vertex (me-vertex) of the semigraph.

In the context of semigraph all vertices belonging to a particular edge are considered as adjacent to one another. Regarding pictorial representations in semigraphs, particular notational convention as followed by Sampathkumar is in order.

An edge  $E$  is represented by a simple open Jordan curve which may be drawn as a straight line as far as possible with its end points as end vertices of  $E$ .

An  $m$ -vertex of an edge  $E$  of a semigraph  $G$  which is not an end vertex of another edge is denoted by a small circle placed on the curve in between the end vertices of  $E$ . An end vertex of an edge which is not an  $m$ -vertex of another edge is represented by a thick dot. When an  $m$ -vertex of an edge  $E$  is also an end vertex of another edge  $\bar{E}$ , we draw a small tangent to the circle at the end of the edge  $\bar{E}$ .

In partial substantiation of the ideas involved in the preceding lines few examples are cited below.

**Example 2.4.1 Family relationship [15]:**

The relationship among the members of a number of families can be represented by a semigraph, where the end vertices of the edges represent the parents and the  $m$ -vertices of edges represent their children, and the parents are treated with equal status in respect of their relationship with their children.

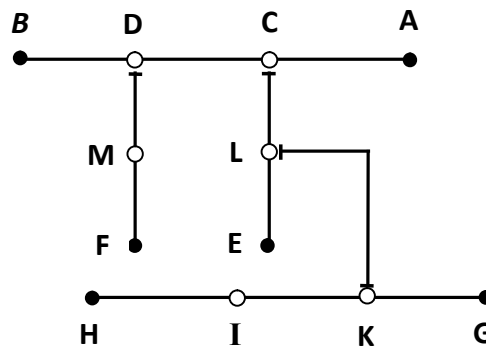


Figure 2.6

Suppose

A and B are the parents of C, D

C and E are the parents of L,

D and F are the parents of a newly born baby M,

L is married to K whose parents are G, H and

K has an unmarried sister I.

This situation is represented by the semigraph in **Figure 2.6** Even, the sex and the age of the members can be represented in such a semigraph by assigning suitably the signs +, -, and integers to the vertices.

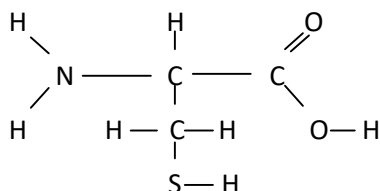
### Example 2.4.2 Chemical semigraph

Chemical semigraph is the generalisation of chemical graph. Chemical semigraphs are useful for depicted chemical compounds in which we consider atoms as vertices and edges are some groups of atoms (i.e. carbon chain, hydroxyl group, ketone group, aldehyde group, carbonyl group, carboxyl group, amino group etc.) and bonds between them. We observed that chemical semigraph is more suitable for represent a chemical compound than by a chemical graph. Molecular structures and corresponding chemical semigraph of some carbon compound and bio chemicals are shown as follows.

#### 1. Structure of Amino Acid:

Name: Cysteine ( $C_3H_7NO_2S$ )

Molecular structure:



-NH <sub>2</sub>	Amino Group
-COOH	Carboxylic Acid Group
-SH	Sulphydryl Group
C-C-C	Carbon-Carbon bond
-H	Hydrogen Atom

Molecular semigraph model of Cysteine ( $C_3H_7NO_2S$ )

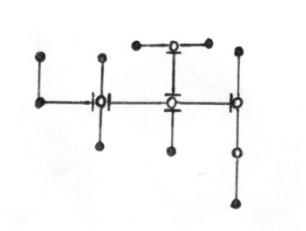


Figure 2.7

2. Structure of Acetamide:

Name: Ethanamide ( $C_2H_5NO$ )

Molecular structure:

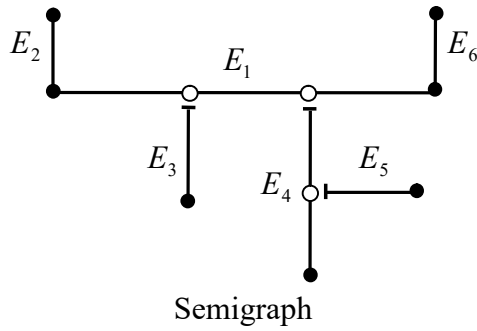
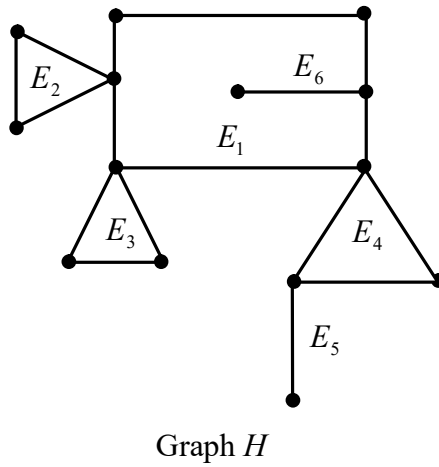


Molecular semigraph model of Ethanamide ( $C_2H_5NO$ )



Figure 2.8

**Example 2.4.3 [15]** A graph  $H$  is considered. A semigraph  $G$  may be constructed from  $H$  such that each edge of  $G$  represents a block of  $H$  and two edges of  $G$  are adjacent if and only if the corresponding blocks in  $H$  have a vertex in common. In **Figure 2.9**, every edge in  $G$  represents a block of  $H$ .



**Figure 2.9**

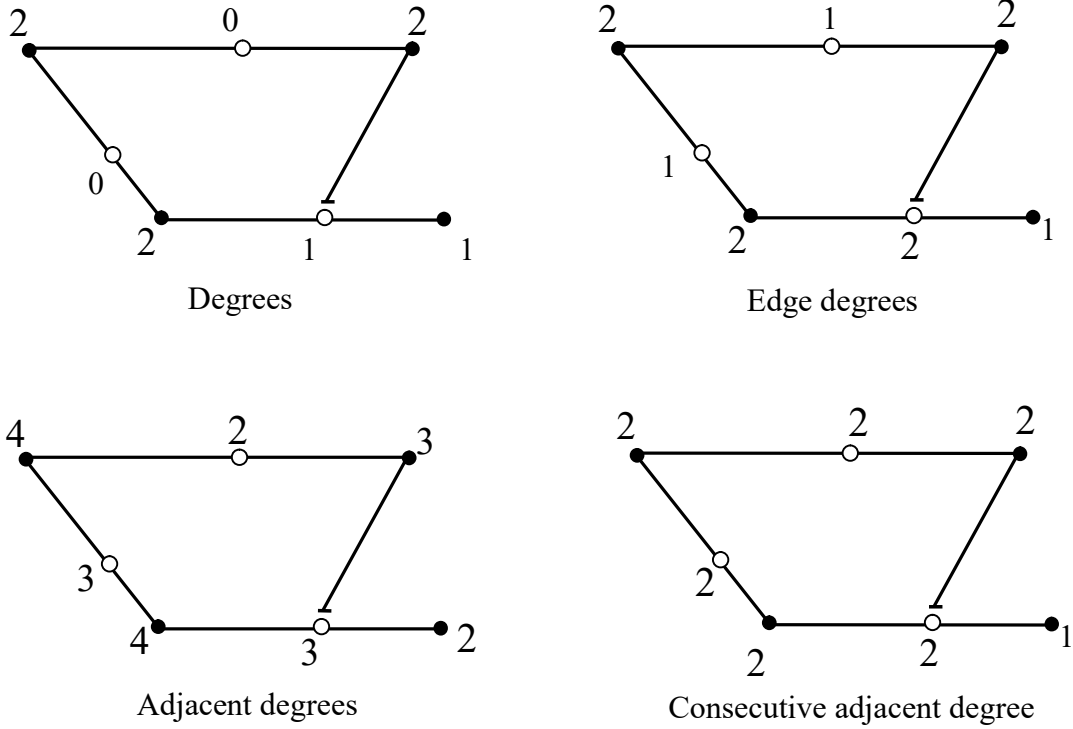
Definition of semigraph provided by Sampathkumar was so rich in structure and form that it gave rise to lots of new concepts parallel to every aspects of graph theory. However, definitions and results relevant only to the present thesis are borrowed from [15, 16, 54] and presented in the following.

**Definition 2.4.2** In a semigraph  $G = (V, X)$ , different types of degrees are defined for a vertex as follows:

- (a) **Degree (or End Degree):**  $deg v$  is the number of edges having  $v$  as an end vertex.
- (b) **Edge degree:**  $deg_e v$  is the number of edges containing  $v$ .
- (c) **Adjacent degree:**  $deg_a v$  is the number of vertices adjacent to  $v$ .

(d) **Consecutive adjacent degree:**  $deg_{ca} v$  is the number of vertices consecutively adjacent to  $v$ .

These are illustrated in **Figure 2.10**.



**Figure 2.10**

Clearly, for any vertex  $v$ ,  $deg v \leq deg_e v \leq deg_a v \leq deg_{ca} v$ . Equality holds for usual graph.

**Proposition 2.4.1**

Let  $G = (V, X)$  be a semigraph of order  $p$  and size  $q$  where,  $V = (v_1, v_2, \dots, v_p)$  and  $X = (E_1, E_2, \dots, E_q)$ . Then,

- (i)  $\sum_{i=1}^p deg v_i = 2q$
- (ii)  $\sum_{i=1}^q deg_e v_i = \sum_{i=1}^q |E_i|$
- (iii)  $\sum_{i=1}^p (deg_a v_i + deg_e v_i) = \sum_{i=1}^q |E_i|^2$
- (iv)  $\sum_{i=1}^p deg_{ca} v_i = 2 \sum_{i=1}^q (|E_i| - 1)$

**Definition 2.4.3** Let  $G = (V, X)$  be a semigraph. Following three graphs associated with  $G$ , have the same vertex set  $V$ :

(a) **End vertex graph (e-Graph)  $G_e$** : Two vertices are adjacent if and only if they are end vertices of an edge in  $G$ .

(b) **Adjacency graph (a-Graph)  $G_a$** : Two vertices are adjacent if and only if they are adjacent in  $G$ .

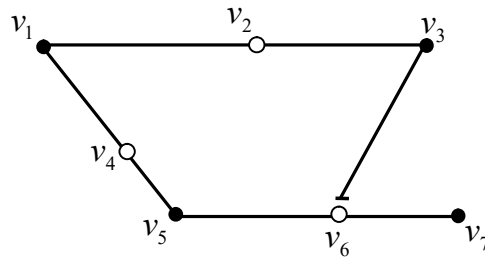
(c) **Consecutive adjacency graph (ca-Graph)  $G_{ca}$** : Two vertices are adjacent if and only if they are consecutively adjacent in  $G$ .

The edge in a semigraph naturally gives rise to the idea of subedges and partial edges which are absent in graph theory.

**Definition 2.4.4** A **subedge (fs-edge)** of an edge  $E=(v_1, v_2, \dots, v_n)$  is a  $k$ -tuple  $E' = (v_{i_1}, v_{i_2}, \dots, v_{i_k})$  where  $1 \leq i_1 < i_2 < \dots < i_k \leq n$  or  $1 \leq i_k < i_{k-1} < \dots < i_1 \leq n$ .

**Definition 2.4.5** A **partial edge (fp-edge)** of an edge  $E=(v_1, v_2, \dots, v_n)$  is a  $(j-i+n)$ -tuple  $E'' = (v_i, v_{i-1}, \dots, v_j)$ , where  $1 \leq i \leq n$ .

**Example 2.4.4** In the semigraph as shown in the **Figure 2.11**  $(v_1, v_3)$  is a subedge of the edge  $(v_1, v_2, v_3)$  whereas,  $(v_5, v_6)$  is a partial edge of the edge  $(v_5, v_6, v_7)$ .



**Figure 2.11**



From the above definitions it is clear that an edge is a subedge (or a partial edge) of itself but a proper subedge (or a proper partial edge) is not an edge. For, otherwise it would contradict the condition that two edges should have at most one vertex in common. Also, a subedge of an edge is a partial edge if and only if any two consecutive vertices in the subedge are also consecutive vertices in the edge.

**Definition 2.4.6** A semigraph  $G' = (V', E')$  is a **subsemigraph** of a semigraph  $G = (V, E)$  if  $V' \subseteq V$  and the edges in  $G'$  are subedges of  $G$ . A **partial subsemigraph** of a semigraph  $G = (V, X)$  is a semigraph whose vertex set is a subset of  $V$  and edges are the partial edges of  $G$ .

A semigraph  $G' = (V', E')$  is said to be an **induced subsemigraph** of a semigraph  $G = (V, X)$ , if the edges  $G'$  of are subedges of  $G$  induced by the vertices in  $V' \subseteq V$ .

A subsemigraph  $G' = (V', E')$  of a semigraph  $G$  is a **spanning subsemigraph** if  $G'$  contains all the vertices of  $G$ .

Using each of the concepts of *fs*-edge and *fp*-edge the definition of walk, trail, path and cycle can be introduced differently for semigraphs.

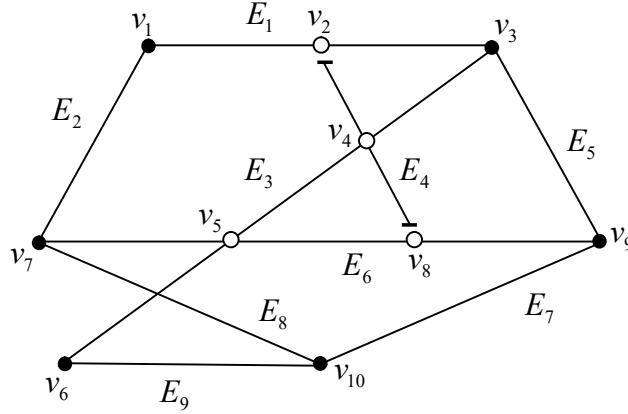
**Definition 2.4.7** A **w-walk (weak walk)** in a semigraph  $G$  is an alternating sequence of vertices and *fs*-edges  $v_0 E_1 v_1 E_2 \dots v_{n-1} E_n v_n$  beginning and ending with vertices, such that  $v_{i-1}$  and  $v_i$  are the end vertices of the *fs*-edge  $E_i$ ,  $1 \leq i \leq n$ . In such a case, it is called a  $v_0 - v_n$  **w-walk**. It is closed if  $v_0 = v_n$ . This walk is called **s-walk (strong walk)** if all its *fs*-edges are *fp*-edges. A *w*-walk is a **w-trail** if any two *fs*-edges in it are distinct. Similarly, **s-trail** can be defined.

A **w-path** (respectively, **s-path**) is a **w-trail** (respectively, *s*-trail) in which all vertices are distinct. A *w*-path is simply referred to as a path.

A **w-cycle** (respectively, **s-cycle**) is a closed **w-path** (respectively, *s*-path).

There is an alternate definition for the *s*-path. A path  $P$  is an **s-path** where any two consecutive vertices are also consecutive vertices of an edge.

**Example 2.4.5** Let us consider the  $v_1 - v_9$   $s$ -path  $v_1 E_1 v_3 E_3 v_6 E_9 v_{10} E_7 v_9$  in **Figure 2.12**, where  $E_1 = (v_1, v_2, v_3)$ ,  $E_3 = (v_3, v_4, v_5, v_6)$ ,  $E_9 = (v_6, v_{10})$  and  $E_7 = (v_{10}, v_9)$ . This path can be written as  $v_1 v_2 v_3 v_4 v_5 v_6 v_{10} v_9$ . But the path  $v_1 v_3 v_4 v_6 v_{10} v_9$  is  $v_1 - v_9$   $w$ -path as because it has the subedges  $(v_1, v_3)$  and  $(v_3, v_4, v_6)$ .



**Figure 2.12**

To define the length of a path as well as a cycle the following definitions become necessary.

Let  $E = (v_1, v_2, \dots, v_m)$  be an edge and  $P : u_0 E_1 u_1 \dots u_{n-1} E_n u_n$  be a  $u_0 - u_n$  path in a semigraph  $G$ . Let us suppose  $E_i = (v_{i_1}, v_{i_2}, \dots, v_{i_k})$  to be a subedge of  $E$  appearing in  $P$ . We say that  $P$  traverses  $E_i$  in  **$r$ -direction** if  $i_1 < i_2 < \dots < i_k$  and  $P$  traverses  $E_i$  in  **$l$ -direction** if  $i_1 > i_2 > \dots > i_k$ . Also, in the travesty of  $P$  from  $u_0$  to  $u_n$ , we say that  $P$  traverses two subedges  $E_1$  and  $E_2$  of  $E$  in the same direction if  $P$  traverses both  $E_1$  and  $E_2$  in either  $r$ -direction or  $l$ -direction.

The **length of a path**  $P : u_0 E_1 u_1 \dots u_{n-1} E_n u_n$  is the number of ordered pairs  $(E_{i-1}, E_i)$ ,  $2 \leq i \leq n$  such that  $E_{i-1}$  and  $E_i$  are not subedges of the same edge traversed in the same direction. Similarly, the **length of a cycle** is defined.

The  **$s$ -distance** between two vertices  $u$  and  $v$  in a semigraph  $G$  is the length of a shortest  $s$ -path between  $u$  and  $v$ . Similarly, the  **$w$ -distance** between  $u$  and  $v$  is

defined. It is observed that the  $s$ -distance between  $u$  and  $v$  is the same as the  $w$ -distance between them. Thus, by distance between  $u$  and  $v$  one should mean the  $s$ -distance or  $w$ -distance and it is denoted by  $d(u, v)$ .

In general, there may be exists a  $w$ -path of length  $k$  between any two vertices of a same edge, but it is not possible in case of an  $s$ -path. For example, if  $E = (v_1, v_2, v_3, v_4, v_5, v_6, v_7)$  is an edge, then  $v_1v_3v_5v_7v_4v_2$  is a  $w$ -path of length of two from  $v_1$  to  $v_2$ , but there is no  $s$ -path of length two between them.

The distance  $d(u, v)$  between the vertices  $u$  and  $v$  in a semigraph  $G$  is the same as the distance between them in the adjacency graph  $G_a$  of  $G$ . However, the length of an  $s$ -path or  $w$ -path  $P$  in  $G$  is not the same as the length of  $P$  in the adjacency graph  $G_a$ .

**Definition 2.4.8** A set  $S$  of vertices in a semigraph  $G$  is **weakly connected** or **strongly connected** according as there exists a weak path or a strong path between any two vertices in  $S$ . Clearly, if  $S$  is strongly connected then it is weakly connected, but not conversely. A semigraph  $G = (V, X)$  is **connected** if  $V$  is connected.

The **removal** of a vertex  $v_i$ ,  $1 \leq i \leq n$  ( $3 \leq n$ ) from an edge  $E = (v_1, v_2, \dots, v_n)$  results in a subedge  $E' = (v_1, v_2, \dots, v_{i-1}, v_{i+1}, \dots, v_n)$  of  $E$ .

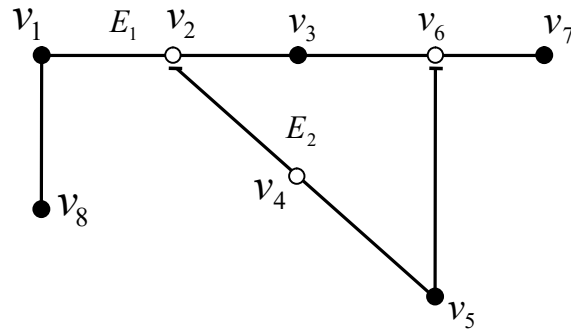
Let  $G = (V, X)$  be a semigraph with  $v \in V$  and  $E \in X$ . The removal of  $v$  from  $G$  results in a semigraph  $G - v = (V', X')$ , where  $V' = V - \{v\}$  and the edges in  $X'$  are defined as follows:

If  $E \in X$  and  $v \notin E$  then  $E \in X'$ .

If  $E \in X$  and  $v \in E$  then  $E - v \in X'$  if and only if  $|E| \geq 3$ . The removal of an edge  $E$  from  $G$  results in a semigraph  $G'' = (V'', X'')$ , where  $V = V''$  and  $X'' = X - \{E\}$ .

**Definition 2.4.9** A **cut vertex** in a semigraph  $G$  is one whose removal increases the components of  $G$  and a **bridge** is such an edge. A **non-separable** semigraph is one that is connected, nontrivial and having no cut vertices.

**Example 2.4.6** In the semigraph shown in **Figure 2.13** below, the vertices  $v_1$  is a cut vertex, whereas  $v_2$  is not a cut vertex. The edge  $E_1 = (v_1, v_2, v_3)$  is a bridge but  $E_2 = (v_2, v_4, v_5)$  is not a bridge.



**Figure 2.13**

**Proposition 2.4.2**

In a semigraph  $G$  the following conditions hold.

- (i) If  $u$  is a vertex in  $G$  then  $(G - u)_a = G_a - u$
- (ii) If  $E$  is an edge in  $G$  with end vertices  $u$  and  $v$  then  $(G - E)_e = G_e - uv$ .

**Proposition 2.4.3** (Characterization of a block)

Let  $G$  be a connected semigraph with at least three vertices. The following statements are equivalent.

- i.*  $G$  is a block.
- ii.* Every two vertices in  $G$  lie on a  $w$ -cycle.
- iii.* Every vertex and a subedge of cardinality two lie on a  $w$ -cycle.
- iv.* Every two subedge of  $G$  of cardinality two lie on a  $w$ -cycle.
- v.* Given two vertices and a subedge of  $G$  of cardinality two, there is a  $w$ -path joining the vertices which contain the subedge.
- vi.* For every three distinct vertices of  $G$  there is a  $w$ -path joining any two of them which contains the third.

- vii. For any three distinct vertices of  $G$ , there is a  $w$ -path joining any two of them which does not contain the third.

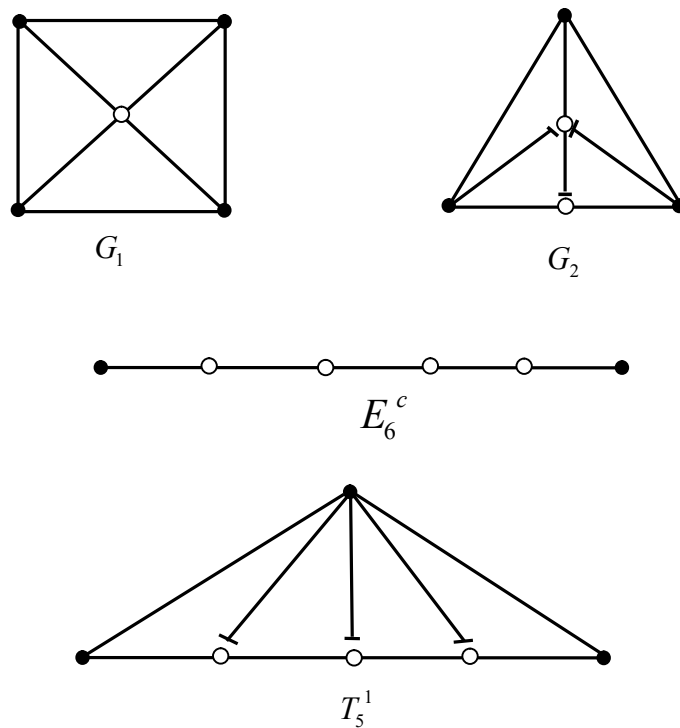
In case of semigraph, there are two types of complete semigraphs one of which is complete and the other is strongly complete.

**Definition 2.4.10** A semigraph  $G$  is **complete** if any two vertices are adjacent.

Further,  $G$  is **strongly complete** if

- (i)  $G$  is complete and
- (ii) Every vertex in  $G$  appears as an end vertex of an edge.

Some examples of complete semigraphs and strongly complete semigraphs are mentioned below. In **Figure 2.14**, the semigraphs  $G_1$  and  $E_6^c$  are complete, whereas the semigraphs  $G_2$  and  $T_5^1$  are strongly complete. E. Sampathkumar [15] denoted the complete semigraph containing only one edge of cardinality  $n \geq 3$  by  $E_n^c$ . He also denoted the strongly complete semigraph of  $n$  vertices with one edge of cardinality  $n - 1$  and all other edges of cardinality two by  $T_{n-1}^1$ .



**Figure 2.14**

Clearly, any strongly complete semigraph is complete, but not conversely.

E. Sampathkumar [15] introduced the concept of bipartition of graphs into semigraphs and defined three types of independent sets and bipartite semigraphs. He also introduced a new concept called edge bipartite semigraph, which is missing in graph theory.

**Definition 2.4.11** A set  $S$  of vertices in a semigraph  $G = (V, X)$  is **independent** if no edge is a subset of  $S$  and  $S$  is  **$e$ -independent** if no two end vertices of an edge belong to  $S$ . The set  $S$  is **strongly independent** if no two adjacent vertices belong to  $S$ . In graphs all these concepts coincide.

Let  $G = (V, X)$  be a semigraph. Then  $G$  is called a **bipartite semigraph** if its vertex set  $V$  can be partitioned into two sets such that they are independent and it is called  **$e$ -bipartite** if the vertex set  $V$  can be partitioned into two sets such that they are  $e$ -independent. The semigraph  $G$  is **strongly bipartite** if the vertex set  $V$  can be partitioned into two sets which are strongly independent.

#### **Proposition 2.4.4**

A semigraph  $G$  is  $e$ -bipartite if and only if, its end vertex graph ( $e$ -graph)  $G_e$  is bipartite.

#### **Proposition 2.4.5**

Let  $G$  be a semigraph having a cycle at least one edge of which has cardinality three. Then  $G$  is bipartite.

**Definition 2.4.12** A semigraph  $G$  is **edge bipartite** if  $G$  has no odd cycle. An edge bipartite semigraph is bipartite, but the converse may not be true.

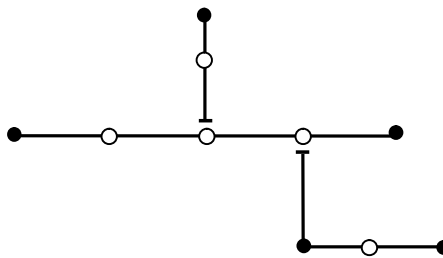
### Proposition 2.4.6

If a semigraph  $G$  is edge bipartite, then it is bipartite. However, the converse is not true.

All these concepts coincide for graphs. It is clear that the only semigraphs which are strongly bipartite are bipartite graphs. Also, every  $e$ -bipartite semigraph is bipartite, but not conversely.

E. Sampathkumar generalized of the concept of trees of graph theory into semigraph and named it as “dendroids”.

**Definition 2.4.13** A **dendroid** is a connected semigraph without  $s$ -cycles (strong cycles) and a **forest** is a semigraph in which every component is a dendroid. The **Figure 2.15** is an example of a dendroid.



**Figure 2.15**

A result due to E. Sampathkumar on dendroids is as follows.

### Proposition 2.4.7

Let  $G$  be a semigraph with  $p$  vertices,  $q$  edges  $E_i$ ,  $1 \leq i \leq q$  and  $k$  components. Then  $G$  contains no cycles if and only if,

$$p + q = \sum_{i=1}^q |E_i| + k$$

**Corollary 2.4.1** A connected semigraph  $G$  with  $p$  vertices and  $q$  edges  $E_i$ ,  $1 \leq i \leq q$  is a dendroid if and only if,

$$p + q = \sum_{i=1}^q |E_i| + 1$$

The concept of ‘‘Covering’’ of graph was also successfully accommodated into the semigraph setting and some results were derived in this direction. As has been the case with any other concept in semigraph, two different types of covering numbers emerged, one relating to vertex and another to edge as follows.

**Definition 2.4.14** In a semigraph  $G$  a vertex  $v$  and an edge  $E$  are incident to each other if  $v \in E$  and in that case,  $v$  and  $E$  are said to cover each other. A set  $S$  of vertices that cover all the edges of a semigraph  $G$  is a **vertex cover** for  $G$ , and  $S$  is an  **$e$ -vertex cover** for  $G$  if  $S$  has only the end vertices of edges.

A set  $L$  of edges covering all the vertices of  $G$  is said to be an **edge cover** of  $G$  and if the edges of  $L$  cover all the end vertices of  $G$  then it is said to be an  **$e$ -edge cover** of  $G$ .

The **vertex covering number**  $\alpha_0 = \alpha_0(G)$  of a semigraph  $G$  is the minimum cardinality of a vertex cover. Similarly, the  **$e$ -vertex covering number**  $\alpha_e = \alpha_e(G)$  of  $G$  is defined.

The **edge covering number**  $\alpha_1 = \alpha_1(G)$  of  $G$  is the minimum cardinality of an edge cover and  **$e$ -edge covering number** of  $G$  is defined similarly.

There are three different types of independence number for a semigraph which are as defined below.

**Definition 2.4.15** The **independence number**  $\beta_0 = \beta_0(G)$  of  $G$  is the maximum cardinality of an independent set of vertices of  $G$  and the  **$e$ -independence number**  $\beta_e = \beta_e(G)$  as well as the **strong independence number**  $\beta_s = \beta_s(G)$  of  $G$  is similarly defined.

A set  $L$  of edges is **independent** if no two edges of  $L$  are adjacent and the set  $L$  is  **$e$ -independent** if no two edges of  $L$  have a common end vertex. The **edge independence number**  $\beta_1 = \beta_1(G)$  of  $G$  is the maximum cardinality of an



independent set of edges, while the ***e*-independence number**  $\beta_{1e} = \beta_{1e}(G)$  is the maximum cardinality of an *e*-independent set of edges of  $G$ .

The following relations can be deduced immediately from the above definitions.

$\alpha_e = \alpha_e(G) = \alpha_0(G_e)$ ,  $\alpha_{1e} = \alpha_{1e}(G) = \alpha_1(G_e)$ ,  $\beta_e = \beta_e(G) = \beta_0(G_e)$  and  $\beta_{1e} = \beta_{1e}(G) = \beta_1(G_e)$ , where  $\alpha_0(G_e)$ ,  $\alpha_1(G_e)$ ,  $\beta_0(G_e)$  and  $\beta_1(G_e)$  are respectively the vertex covering number, edge covering number, vertex independence number and edge independence number of the *e*-graph  $G_e$  associated with the semigraph  $G$ . Also, we have,  $\beta_s = \beta_s(G) = \beta_0(G_a)$ , where  $\beta_0(G_a)$  denote the vertex independence number of the *a*-graph  $G_a$  associated with the semigraph  $G$ .

### Proposition 2.4.8

For any semigraph  $G$ ,  $\alpha_0 \leq \alpha_e$  and  $\beta_s \leq \beta_e \leq \beta_0$ .

### Proposition 2.4.9

Let  $G = (V, X)$  be a semigraph with  $p$  vertices and  $q$  edges  $E_i$ ,  $1 \leq i \leq q$ . Then

- (i)  $\alpha_0 + \beta_0 = p$
- (ii) For a semigraph  $G$  with no vertex of degree zero,  
 $\alpha_e + \beta_e = p$ .

A similar result is believed to be true for edge bipartite semigraph and has been presented as a conjecture by Sampathkumar as given below.

**Conjecture 2.4.1** Let  $G = (V, X)$  be an edge bipartite semigraph. Then,

$$\alpha_e(G) = \beta_{1e}(G)$$

### Proposition 2.4.10

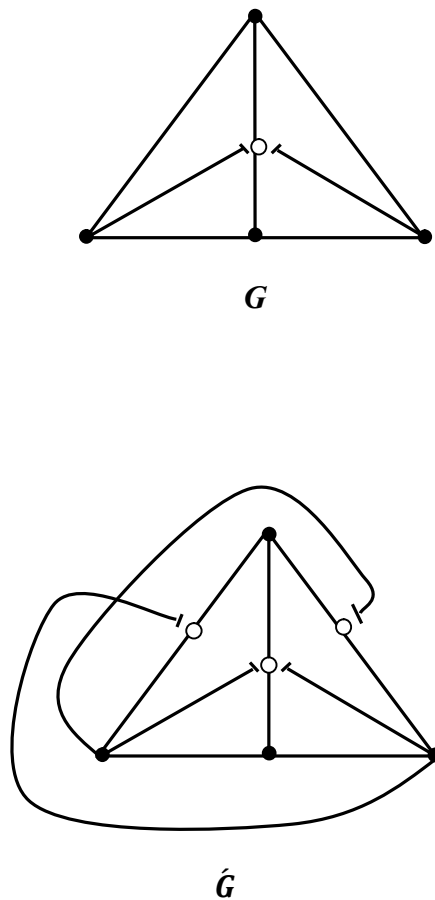
If  $G$  is a semigraph of order  $p$  having no vertices of degree zero, then

$$\alpha_{1e} + \beta_{1e} = p$$

In [15] we also come across planarity of semigraph and find Euler's Polyhedral formula for planar semigraphs.

**Definition 2.4.16** A semigraph is said to be **embedded** in a surface when it is drawn on it so that no two edges intersect at a point not representing a vertex of the semigraph on the surface.

A **planar** semigraph is one which can be embedded in a plane. In the **Figure 2.16**, the semigraph  $G$  is planar, but the semigraph  $G'$  is not planar.



**Figure 2.16**

The regions defined by a planar embedding semigraph are called its faces. The unbounded region is called the **exterior face** of the embedding.

Coloring is another important aspect of graph theory that has been studied by Sampathkumar in the semigraph setting. Three types of vertex coloring and two types of edge coloring are introduced and corresponding vertex coloring numbers and edge coloring numbers are defined.

**Definition 2.4.17** A **coloring** of a semigraph  $G$  is an assignment of colors to its vertices such that not all vertices in a same edge colored the same.

A **strong coloring** (an  **$e$ -coloring**) of  $G$  is a coloring of vertices so that no two adjacent vertices (end vertices of an edge) are colored the same. As  **$n$ -coloring** ( **$n$ -strong coloring**,  **$n$ - $e$ -coloring**) uses  $n$  colors and partitions the vertex set of  $G$  into  $n$  respective color classes, each class consisting of vertices of the same color.

The **chromatic number**  $\chi = \chi(G)$  of  $G$  is the minimum number of colors needed in any coloring of  $G$ . Similarly, we define the **strong chromatic number**  $\chi_s = \chi_s(G)$  and the  **$e$ -chromatic number**  $\chi_e = \chi_e(G)$  of  $G$ . Clearly a strong coloring is an  $e$ -coloring and an  $e$ -coloring is a coloring.

**Proposition 2.4.11**

For any semigraph of order  $p$ ,

$$\chi \leq \chi_e \leq \chi_s \leq p.$$

**Proposition 2.4.12**

For any semigraph  $G$ ,  $\chi_s(G) \leq \chi_e(G) + m$ , where  $m$  is the number of middle vertices of  $G$ .

**Proposition 2.4.13**

Let  $G$  be a semigraph with at least one edge. Then  $G$  is

- (i) Bipartite if and only if,  $\chi(G) = 2$
- (ii)  $e$ -bipartite if and only if,  $\chi_e(G) = 2$  and
- (iii) strongly bipartite if and only if,  $\chi_s(G) = 2$

**Definition 2.4.18** Let  $G = (V, X)$  be a semigraph with  $\chi(G) = n$ . A  $\chi(G)$ -**partition** of  $G$  is a partition  $\{V_1, V_2, \dots, V_n\}$  of  $V$  into independent sets. Similarly, a  $\chi_e(G)$ -**partition** and a  $\chi_s(G)$  -**partition** of  $G$  are defined.

**Definition 2.4.19** A partition  $\{V_1, V_2, \dots, V_n\}$  of  $V$  is **complete** if for any  $V_i$  and  $V_j$ ,  $i \neq j$ ,  $V_i \cup V_j$  contains an edge.

**Proposition 2.4.14**

The partitions  $\chi(G)$ ,  $\chi_e(G)$  and  $\chi_s(G)$  of  $G$  are all complete.

**Proposition 2.4.15**

If  $G$  is a planar semigraph then,  $\chi(G) \leq \chi_e(G) \leq 5$ .

**Proposition 2.4.16**

For any semigraph  $G$  of order  $p$ ,

- (i)  $\frac{p}{\beta_0} \leq \chi_e(G) \leq p - \beta_0 + 1$ ,
- (ii)  $\frac{p}{\beta_e} \leq \chi_e(G) \leq p - \beta_e + 1$  and
- (iii)  $\frac{p}{\beta_s} \leq \chi_s(G) \leq p - \beta_s + 1$

**Proposition 2.4.17**

For any semigraph  $G$ ,

$$\chi(G) \leq \max \delta_e(G') + 1,$$

where, the maximum is taken over all edge induced subsemigraphs  $G'$  of  $G$  and  $\delta_e(G')$  denotes the minimum edge degree of a vertex  $v$  in  $G'$ .

**Corollary 2.4.2** For any semigraph  $G$ ,

$$\chi(G) \leq \Delta_e(G) + 1,$$

where,  $\Delta_e(G)$  denotes the maximum edge degree of a vertex  $v$  in  $G$ .

**Corollary 2.4.3** For any semigraph  $G$  of order  $p$ ,

$$\beta_0(G) \leq p/\Delta_e(G) + 1$$

**Corollary 2.4.4** If  $\alpha_0(G)$  is the point covering number of  $G$ , then

$$\alpha_0(G) \leq \frac{p\Delta_e(G)}{\Delta_e(G)} + 1$$

**Proposition 2.4.18**

For any semigraph  $G$ ,

$$\chi_e(G) \leq \max \delta(G'_e) + 1,$$

where, the maximum is taken over all edge induced subsemigraphs  $G'_e$  of  $G_e$ .

**Corollary 2.4.5** For any semigraph  $G$ ,

$$\chi_e(G) \leq \Delta(G) + 1$$

**Proposition 2.4.19**

For any semigraph  $G$ ,

$$\chi_s(G) \leq \max \delta_a(G') + 1$$

Where the maximum is taken over all the edge induced subsemigraphs  $G'$  of  $G$  and  $\delta_a(G')$  denotes the minimum adjacent degree of a vertex  $v$  in  $G'$ .

**Definition 2.4.20** An **edge coloring** of a semigraph  $G$  is an assignment of colors to its edges so that no two edges with a common vertex are colored the same.

An  **$e$ -edge coloring** of a semigraph  $G$  is an assignment of colors to its edges so that no two edges with a common end vertex are colored the same. An  **$n$ -edge coloring** of  $G$  uses  $n$  colors.

The **edge chromatic number** (or **chromatic index**)  $\chi'(G)$  of a semigraph  $G$  is the minimum number  $n$  for which  $G$  has an  $n$ -edge coloring. An  **$e$ -edge chromatic number**  $\chi'_e(G)$  of  $G$  is the minimum number of colors needed in an  $e$ -edge coloring of  $G$ . Clearly,  $\chi'_e(G) \leq \chi'(G)$  for any semigraph  $G$  and  $\chi'_e(G) = \chi'(G_e)$  where  $\chi'(G_e)$  is the edge chromatic number of the  $e$ -graph  $G_e$  corresponding to the semigraph  $G$ . If  $G$  is a graph then,  $\chi'_e(G) = \chi'(G)$ .

**Definition 2.4.21** A set  $S$  of edge in a semigraph  $G$  is said to form an **edge clique** if any two edge in  $S$  are adjacent. The **edge clique number**  $\omega_e(G)$  of  $G$  is the maximum cardinality of an edge clique in  $G$ .

If  $G$  is a graph, we observe that  $\omega_e(G) = \Delta(G)$ , the maximum degree of  $G$ .

**Proposition 2.4.20**

If  $G$  is an edge bipartite semigraph, then  $\omega_e(G) = \Delta_e(G)$  where,  $\Delta_e(G)$  denotes the maximum edge degree of  $G$ .

**Proposition 2.4.21**

If  $G$  is an edge bipartite semigraph, then

- (i)  $\chi'(G) = \omega_e(G) = \Delta_e(G)$
- (ii)  $\chi'_e(G) = \Delta(G)$

**Corollary 2.4.6** For any dendroid  $G$ ,  $\chi'(G) = \Delta_e(G)$ .

**Proposition 2.4.22** (Vizing-Type Theorem for  $e$ -edge Chromatic Number)

For any semigraph  $G$ ,

$$\Delta(G) \leq \chi'_e(G) \leq \Delta(G) - 1.$$

**Proposition 2.4.23**

For every semigraph  $G$ ,  $\chi'(G) \geq \omega_e(G)$ .

**Conjecture 2.4.2** For any semigraph  $G$ ,  $\chi'(G) \leq \omega_e(G) + 1$ .

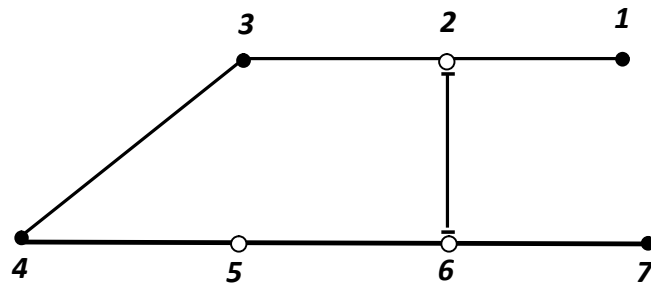
The semigraphs like graphs can be classified into two classes. A semigraph  $G$  is said to belong to Class I if  $\chi'(G) = \omega_e(G)$ , and to Class II if  $\chi'(G) = \omega_e(G)$ . Again, a semigraph  $G$  belongs to Class  $I_e$ , if  $\chi'_e(G) = \Delta(G)$  while  $G$  belongs to Class  $II_e$  if  $\chi'_e(G) = \Delta(G) + 1$ .

Domination is one of the important areas Graph Theory introduced by C. Berge in 1985 and called as external stability. The concept of domination in semigraph provides a lot of scope for theoretical development and applications. There are various types of domination in semigraph like a-domination, ca-domination, ev-domination, etc.

**Definition 2.4.22  $\alpha$ -Domination [16]:** Let  $S = (V, X)$  be a semigraph. A subset  $D$  of  $V$  is called a-dominating set of  $S$  if for all  $v \in V - D$  there exist  $u \in D$  such that  $u$  and  $v$  are adjacent.

The minimum cardinality of a-dominating set of  $S$  is called the  **$\alpha$ -domination number** of  $S$  and is denoted by  $\gamma_\alpha$ .

**Example 2.4.7** If  $S = (V, X)$  be a semigraph with vertex set  $V = \{1, 2, 3, 4, 5, 6, 7\}$  and edge set  $X = \{(1,2,3), (3,4), (2,6), (4,5,6,7)\}$  as shown in **Figure 2.17**. Then  $D = \{3, 4\}$  is a-dominating set of  $S$ . It is also a minimum a-dominating set of  $S$ . Therefore  $\gamma_\alpha(S) = 2$ .

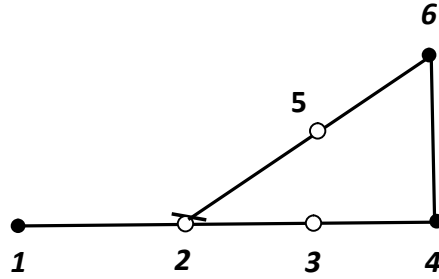


**Figure: 2.17**

**Definition 2.4.23  $ca$ -Domination [16]:** A subset  $D$  of  $V(S)$  is called an ca-dominating set if for every  $v \in V - D$ , there exist a  $u \in D$  such that  $u$  and  $v$  are consecutive vertices of an edge.

The minimum cardinality of a  $ca$ -dominating set is denoted by  $\gamma_{ca}(S)$ , and called the  $ca$ -domination number of  $S$ .

**Example 2.4.8** If  $S = (V, X)$  be a semigraph with vertex set  $V = \{1, 2, 3, 4, 5, 6\}$  and edge set  $X = \{(1,2,3,4), (4,6), (2,5,6)\}$  as in **Figure 2.18**. Then  $D = \{2, 6\}$  is the  $ca$ -dominating set of  $S$  with minimum cardinality. Therefore  $\gamma_{ca}(S) = 2$ .



**Figure: 2.18**

**Definition 2.4.24  $ev$ -Domination [16]:** A subset  $D$  of  $V(S)$  is called an end vertex dominating set if for every  $u \in V - D$ , there exist a  $v \in D$  such that  $v$  is an end vertex of an edge containing  $u$ .

The minimum cardinality of an  $ev$ -dominating set of  $S$  is denoted by  $\gamma_{ev}(S)$ .

**Example 2.4.9** If  $S = (V, X)$  be a semigraph with vertex set  $V = \{1, 2, 3, 4, 5, 6\}$  and edge set  $X = \{(1,2,3,4), (4,6), (2,5,6)\}$  as shown in **Figure 2.18**. Then  $D_1 = \{2, 4\}$  or  $D_2 = \{4, 6\}$  are the  $ev$ -dominating set of  $S$  with minimum cardinality. Therefore  $\gamma_{ev}(S) = 2$ .

**Definition 2.4.25 Signed semigraph [43]:**

**$e$ -Signed semigraph:** Suppose  $S(V, E)$  be a signed semigraph. In  $S$ , the edge with odd number of middle vertices (or  $m$ -vertices) is assigned negative sign and the edge with even number of  $m$ -vertices or without  $m$ -vertices is assigned positive sign. Then  $S$  is called an  $e$ -signed semigraph.



**$v$ -Signed semigraph:** A semigraph  $S(V, E)$  is called  $v$ -signed, if sign of every end vertex of  $S$  is assigned either positive or negative sign according as consecutive adjacent degree of the end vertex is even or odd.

**$ve$ -Signed semigraph:** A semigraph  $S(V, E)$  is called  $ve$ -signed, if every end vertex and every edge of  $S$  is assigned either positive or negative sign.

Matrix representations of semigraphs is one of the most important concepts introduced by Sampathkumar in his book. The adjacency matrix, the incidence matrix, the consecutive adjacency matrix and the 3-matrix of semigraph are defined. The incidence matrix, together with the consecutive adjacency matrix determine a semigraph uniquely. Also, the 3-matrix of a semigraph  $G$  determines  $G$  uniquely.

**Definition 2.4.26 The adjacency matrix [15]:**

Let  $G = (V, X)$  be a semigraph with  $V = \{v_1, v_2, \dots, v_p\}$  and  $X = \{e_1, e_2, \dots, e_q\}$  then, the adjacency matrix  $A = A(G) = [a_{ij}]$  of  $G$  is the  $p \times p$  matrix in which  $a_{ij} = 1$  if  $v_i$  is adjacent to  $v_j$  and  $a_{ij} = 0$  otherwise.

Clearly,  $A(G) = A(G_a)$ , i.e., the adjacency matrix of  $G$  is the same as that of its adjacency matrix of a semigraph.

**Proposition 2.4.24** The  $i, j$  entry in the matrix  $A^n$  is the number of walks of length  $n$  from  $v_i$  to  $v_j$  in  $G$ .

**Corollary 2.4.7** If  $v_i$  and  $v_j$  are non-adjacent, then the  $i, j$  entry in  $A^2$  is the number of paths of length two from  $v_i$  to  $v_j$  and the  $i, j$  entry in  $A^2$  is the adjacent degree  $deg_a v_i$  of  $v_i$ .

**Corollary 2.4.8** If  $G$  is connected, the distance between  $v_i$  and  $v_j$ ,  $i \neq j$ , is the least integer  $n$  for which the  $i, j$  entry  $A^n$  is not zero.

Note that the adjacency matrix  $A$  determines the adjacency graph  $G_a$  of  $G$  uniquely, but it does not determine  $G$  uniquely.

**Definition 2.4.27 The incidence matrix [15]:**

The incidence matrix  $B = [b_{ij}]$  of  $G$  is the  $p \times p$  matrix where  $b_{ij} = 1$  if  $v_i$  and  $e_j$  are incident and  $b_{ij} = 0$  otherwise. Clearly, the sum of the entries in the  $i^{\text{th}}$  column gives the dimension of the edge  $e_i$  i.e., the number of vertices in  $e_i$ . The incidence matrix also does not determine the semigraph uniquely.

The following proposition characterizes the incidence matrix of a semigraph.

**Proposition 2.4.25** A  $p \times p$  matrix  $B = [b_{ij}]$  is the incidence matrix of a semigraph  $G$  if and only if,

- i.  $q \leq \binom{p}{2}$
- ii. the sum of entries in each column is at least two and
- iii. for any  $i, j, i \neq j, 1 \leq i, j \leq q$  and for at most one  $r, b_{ri} = b_{rj} = 1$  where  $1 \leq r \leq p$ .

**Definition 2.4.28 The consecutive adjacency matrix [15]:**

The consecutive adjacency matrix  $A_{ca} = [c_{ij}]$  of a semigraph  $G$  is the  $p \times p$  matrix where  $c_{ij} = 1$  if  $v_i$  and  $v_j$  are consecutive adjacent vertices in  $G$  and  $c_{ij} = 0$  otherwise.

Clearly,  $A_{ca}$  is the adjacency matrix of the consecutive adjacency graph  $G_{ca}$  of  $G$ . The matrix  $A_{ca}$  also does not determine the semigraph uniquely. The consecutive adjacency matrix  $A_{ca}$  together with the incidence matrix  $B$  of a semigraph  $G$  determines  $G$  uniquely. While the incidence matrix gives the vertices in each edge, the consecutive adjacency matrix determines the order of the vertices in each edge. Thus, we can associate with each semigraph, a pair of  $(0, 1)$ -matrices uniquely and conversely, with some specified pair of  $(0, 1)$ -matrices, we can associate a semigraph uniquely.

**Proposition 2.4.26** Let  $A = [a_{ij}]$  and  $B = [b_{ij}]$  be two  $(0, 1)$ -matrices of orders  $p \times p$  and  $p \times q$  respectively. Then they determine a  $(p, q)$ -semigraph  $G$  uniquely if and only if, the following conditions hold.

- i.  $B$  is the incidence matrix of a semigraph  $G$
- ii.  $A$  is a symmetric matrix.
- iii. For each edge  $e$  of cardinality  $k$  corresponding to a column in  $B$ , the vertices of  $e$  can be labelled as say,  $v_1, v_2, \dots, v_k$  such that there are  $2(k - 1)$  entries of 1 in  $A$  given by  $a_{jj+1} = a_{j-1j} = 1, 1 \leq j \leq k - 1$ .
- iv. All other entries in  $A$  are zero.

**Definition 2.4.29 3-Matrix representation of a semigraph [15]:**

Given a semigraph  $G = (V, X)$  on  $p$  vertices and with  $q$  edges, we can represent it uniquely by a  $p \times p$  matrix  $C(G) = (c_{mn})$  as follows:

Each  $c_{mn}$  is a 3-tuple of non-negative integers  $(k: i, j)$  where  $0 \leq k \leq q, 0 \leq i \leq r, 0 \leq j \leq r$  and  $r$  is the maximum cardinality of an edge in  $G$ .

Let  $V = (v_1, v_2, \dots, v_p)$  and  $X = (e_1, e_2, \dots, e_q)$ . Then the entries  $c_{mn}$  of the matrix  $C(G)$  are defined as follows:

$c_{mn} = (0: 0, 0)$  if either  $m = n$ , or  $v_m$  and  $v_n$  are non-adjacent.

$c_{mn} = (k: i, j)$  if  $v_m$  and  $v_n$  lie on the edge  $e_k, i < j$  and  $v_m$  lies in the  $i^{\text{th}}$  position and  $v_n$  lies in the  $j^{\text{th}}$  position in the edge  $e_k$ . A characteristic of the 3-matrix of a semigraph is given below.

**Proposition 2.4.27** A  $p \times p$  matrix  $C = (c_{mn})$  where each  $c_{mn}$  is a 3-tuple  $(k: i, j)$  of non-negative integers  $k, i, j$  with  $1 \leq k \leq \binom{p}{2}$  and  $1 \leq i \leq j \leq p$  is the 3-matrix of a  $(p, q)$ -semigraph  $G$  if and only if, the following hold:

- i. All the diagonal entries are  $(0: 0, 0)$ .
- ii. Each 3-tuple either contains all zeros or all non-zero entries.

- iii. Let  $S_1 = \{1, 2, \dots, q\}$  and  $S_2 = \{2, 3, \dots, p\}$ . Then for each  $k$  in  $S_1$  there exists a  $j_k$  in  $S_2$  satisfying the following:
- $\sum \binom{j_k}{2} \leq \frac{p(p-1)}{2}$
  - The upper diagonal entries include all the  $\binom{j_k}{2}$  integers  $(k: i, j)$ ,  
 $1 \leq i < j \leq j_k$  for each  $k$ .
- iv. If  $c_{mn} = (k: i, j)$ , then  $c_{nm} = (k: j_k - j + 1, j_k - i + 1)$ .

Adjacency matrix associated with a semigraph defined by the authors C. M. Deshpande and Y. S. Gaidhani [10] as follows:

**Definition 2.4.30 Adjacency matrix associated with a semigraph:**

If  $G(V, X)$  be a semigraph with vertex set  $V = \{1, 2, 3, \dots, m\}$  and edge set  $X = \{e_1, e_2, e_3, \dots, e_n\}$  where  $e_j = (i_1, i_2, i_3, \dots, i_{k_j})$ ,  $j = 1, 2, 3, \dots, n$  and  $i_1, i_2, i_3, \dots, i_{k_j}$  are distinct elements of  $V$ . Adjacency matrix,  $A$ , of  $G(V, X)$  is a  $m \times m$  matrix whose entries are given by

$$a_{i,j} = \text{cardinality of } fp\text{-edge}(v_i, v_j) - 1 \quad ; \text{ if } v_i, v_j \text{ are adjacent}$$

$$= 0 \quad ; \text{ otherwise.}$$

As every  $p$ -edge of cardinality  $\geq 2$  belongs to exactly one  $f$ -edge of  $G$ , the above matrix is well defined. We label the rows and columns of  $A$  as  $1, 2, 3, \dots, m$ ; the same as vertex set of  $G$ .

Also, a  $m \times m$  matrix  $A$  is said to be semigraphical if there exists a semigraph  $G$  on  $m$  vertices having adjacency matrix as  $A$ .

Again, in the year 2017, Y. S. Gaidhani, C. M. Deshpande and B.P. Athawale [65] defined adjacency matrix associated with a semigraph in another way as follows:

**Definition 2.4.31 Adjacency matrix associated with a semigraph:**

Let  $G(V, X)$  be a semigraph with vertex set  $V = \{v_1, v_2, \dots, v_p\}$  and edge set  $X = \{e_1, e_2, \dots, e_q\}$ . The Adjacency matrix of  $G(V, X)$  is a  $p \times p$  matrix  $A = [a_{ij}]$  defined as follows:

1. For every edge  $e_i$  of  $X$  of cardinality, say  $k$ , let  $e_i = (i_1, i_2, i_3, \dots, i_k)$  such that  $i_1, i_2, i_3, \dots, i_k$  are distinct vertices in  $V$ , for all  $i_r \in e_i; r = 1, 2, \dots, k$ 
  - (a)  $a_{i_1 i_r} = r - 1$
  - (b)  $a_{i_k i_r} = k - r$
2. All the remaining entries of  $A$  are zero.

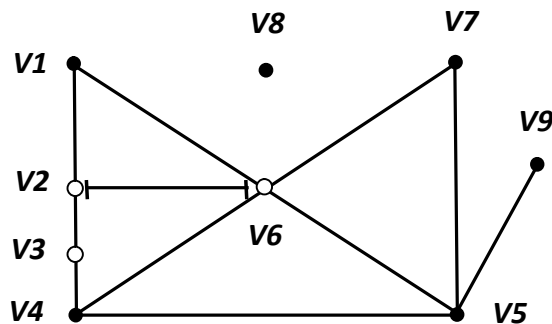
On the other hand, a  $p \times p$  matrix  $M$  is said to be semigraphical if there exists a semigraph  $G$  on  $p$  vertices with adjacency matrix equal to  $M$ .

**Example 2.4.10** Consider a semigraph  $G = (V, X)$ , in **Figure 2.19** where

$V = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$  and

$X = \{(1, 2, 3, 4), (4, 5), (1, 6, 5), (4, 6, 7), (5, 7), (2, 6), (5, 9)\}$ .

Here vertices 1, 4, 5, 6, 7 and 9 are the end vertices, 3 is a middle vertex, 2 and 6 are the middle-end vertices and 8 is an isolated vertex.



**Figure: 2.19**

The adjacency matrix of  $G$  is

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

V. Nikiforov [60] defined the energy of a general matrix (any size) as the summation of the singular values of that matrix. Analogy with this definition, Y. S. Gaidhani et al. [64] introduced energy of semigraph as follows.

**Definition 2.4.32 Energy of a semigraph:**

Let  $G(V, X)$  be a semigraph having order  $p$  and size  $q$ . If  $A$  be the adjacency matrix of  $G$  which is defined by Y. S. Gaidhani, *et. al.* [65]. Then, energy of a semigraph  $G$  is defined as the summation of the singular values of  $A$ .

**Lemma 2.4.1** If  $A(G)$  is the adjacency matrix of a semigraph  $G$  on  $p$  vertices and are the eigenvalues of  $AA^T$ , then  $\sum_{i=1}^p \mu_i = 2 \sum_{e \in X} (1^2 + 2^2 + 3^2 + \dots + k_e^2)$ .

**Theorem 2.4.1** For a semigraph  $G$  on  $p$  vertices

$$\sqrt{2 \sum_{e \in X} (1^2 + 2^2 + 3^2 + \dots + k_e^2)} \leq E(G) \leq \sqrt{2p \sum_{e \in X} (1^2 + 2^2 + 3^2 + \dots + k_e^2)}$$

**Theorem 2.4.2** For a semigraph  $G$  on  $p$  vertices

$$E(G)^2 \geq 2 \sum_{e \in X} (1^2 + 2^2 + 3^2 + \dots + k_e^2) + p(p-1)\Delta^{1/p}$$

where  $\Delta = \det(AA^T)$ .

**Theorem 2.4.3** If  $G$  is a Semigraph on  $p$  vertices having largest singular value  $\sigma_1$  and second largest singular value  $\sigma_2$ , then

$$E(G) \geq \sigma_1 + \frac{2p \sum_{e \in X} (1^2 + 2^2 + 3^2 + \dots + k_e^2) - \sigma_1^2}{\sigma_2}$$

**Theorem 2.4.4** The energy  $E(G)$  of semigraph  $G$  is never the square root of an odd integer.

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