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Unit – 4 ⇝ Spectral Graph Theory

Introduction

→ This unit focused on

→ **Key Question:** How can we analyze the structure of a graph using matrices and the spectrum of associated operators?

→ We learned about the **Adjacency Matrix**, **Degree Matrix**, and the **Laplacian Matrix**, which encode structural information about graphs in algebraic form.

→ We explored the **Cut-Set Matrix** to understand graph partitions and connectivity patterns.

→ We also studied **Eigenvalues and Eigenvectors** of these matrices to reveal deep properties of graphs, such as connectivity, expansion, and clustering.

→ These tools are powerful in real-world applications like ranking in networks, image segmentation, and machine learning on graphs.

Method – 1 ⇝ Matrix Representation of graphs

Definition: Let $G = (V, E)$ be a graph with n vertices and without parallel edges. The adjacency matrix of graph $G = (V, E)$ is denoted as A or $A(G)$ and is defined as $n \times n$ matrix $A = [a_{ij}]$ whose elements a_{ij} are given as follows:

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

Definition: Let $G = (V, E)$ be a graph with n vertices. The degree matrix of graph $G = (V, E)$ is denoted as D or $D(G)$ and is defined as $n \times n$ diagonal matrix $D = [d_{ij}]$ whose elements d_{ij} are given as follows:

$$d_{i,j} = \begin{cases} d(v_i), & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

Where, $d(v_i)$ is the degree of vertex v_i.

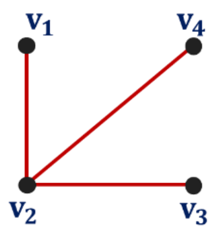
Definition: Let $G = (V, E)$ be a simple graph with n vertices. The Laplacian matrix of graph $G = (V, E)$ is denoted as $L(G)$ and is defined as $n \times n$ matrix $L = [l_{ij}]$ whose elements l_{ij} are given as follows:

$$d_{i,j} = \begin{cases} -1, & \text{if } v_i \text{ is adjacent to } v_j \\ d(v_i), & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

Where, $d(v_i)$ is the degree of vertex v_i.

→ Equivalently $L = D - A$, where D is the degree matrix, and A is the graph's adjacency matrix.

Example: Find Laplacian matrix of the following graph.



Solution: Here first we find adjacency matrix of the given graph.

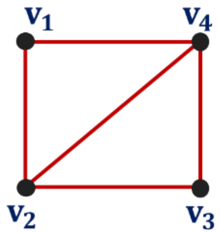
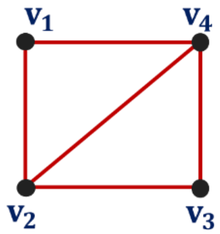
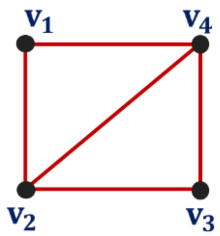
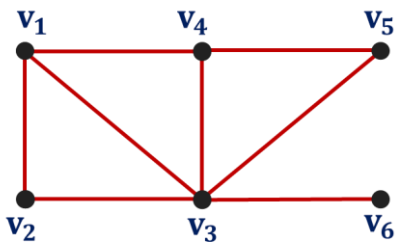
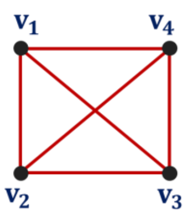
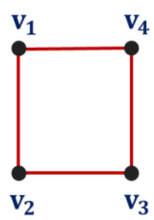
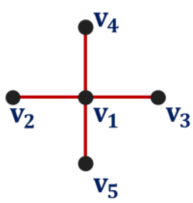
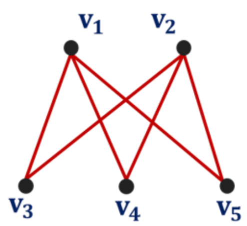
$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}.$$

Now we find Degree matrix of the given graph.

$$D = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Hence, Laplacian matrix $L = D - A = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}.$

Example of Method-1: Matrix Representation of Graph

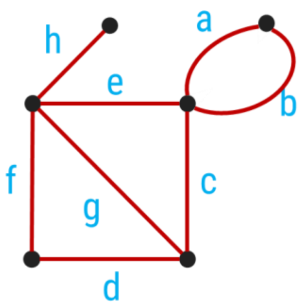
C	1	Find an adjacency matrix for the following graph. 
C	2	Find the degree matrix for the following graph. 
C	3	Find the Laplacian matrix for the following graph. 
C	4	Find the Laplacian matrix for the following graph. 
C	5	Find the Laplacian matrix for the following graph.  K_4  C_4  S_5  $K_{2,3}$
H	6	Find the Laplacian matrix of $\mathbf{K_5}$.
H	7	Find the Laplacian matrix of $\mathbf{C_5}$.
H	8	Find the Laplacian matrix of $\boldsymbol{K_{4,4}}$.

Method – 2 ⇝ Cut-set Matrix and it's properties

Definition: Let $G = (V, E)$ be a graph. The cut-set matrix of graph $G = (V, E)$ is denoted as C or $C(G)$, in which the rows correspond to the cut-sets and the columns to the edges of the graph and is defined as matrix $C = [c_{ij}]$ whose elements c_{ij} are given as follows:

$$c_{i,j} = \begin{cases} 1, & \text{if } i^{th} \text{ cutset contains } j^{th} \text{ edge} \\ 0, & \text{otherwise} \end{cases}$$

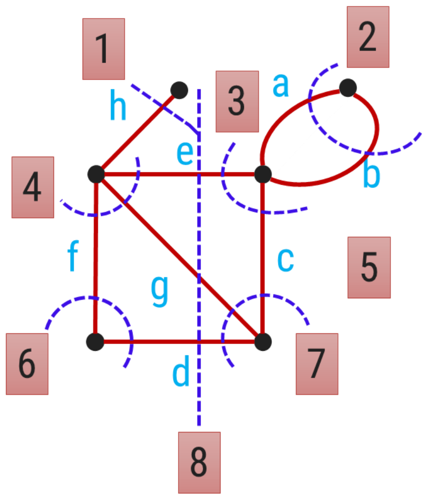
Example: Find Cut-Set Matrix for Following Graph



Solution: Here, given graph have 8 cut set and 8 edges.

That means we get 8×8 cut-set matrix of given graph.

$$C = [c_{ij}]_{8\times 8} = \begin{array}{c} \\ 1\\2\\3\\4\\5\\6\\7\\8 \end{array} \begin{array}{c} \begin{array}{cccccccc} a & b & c & d & e & f & g & h \end{array} \\ \begin{bmatrix} 0&0&0&0&0&0&0&1\\ 1&1&0&0&0&0&0&0\\ 0&0&1&0&1&0&0&0\\ 0&0&0&0&1&1&1&0\\ 0&0&1&0&0&1&1&0\\ 0&0&0&1&0&1&0&0\\ 0&0&1&1&0&0&1&0\\ 0&0&0&1&1&0&1&0 \end{bmatrix} \end{array}$$



Definition: Let $G = (V, E)$ be a graph with n vertices and e edges. The fundamental cut-set matrix of graph G is $n - 1 \times e$ denoted as C_f, which sub matrix of C such that the rows correspond to the set of fundamental cut-sets with respect to some spanning tree.

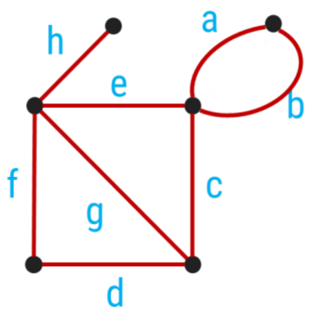
A fundamental cut-set matrix C_f can also be partitioned into two sub matrices, one of which is an identity matrix I_{n-1}, of order $n - 1$. That is

$$C_f = [C_c | I_{n-1}].$$

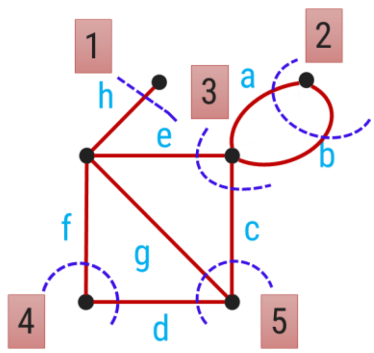
Properties:

1. The last $n-1$ columns of fundamental cutset matrix forming the identity matrix correspond to the $n-1$ branches of the spanning tree.
2. The first $e-n+1$ columns forming C_c correspond to the chords.
3. Rank of cut-set matrix = Rank of the fundamental cutset matrix = Rank of graph.

Example: **Find Fundamental Cut-Set Matrix for the Following Graph**



Solution:



→ First we consider any spanning tree of given graph.

→ Say {h, e, f, g, a}.

→ Now, we find all of its fundamental cut sets.

→ Here, graph have 5 fundamental cut set and 8 edges. As graph have 5 branches and 3 chord.

→ That means we get 5×8 fundamental cut-set matrix of given graph.

→ Hence, in fundamental cutset matrix the last 5 columns forming the identity matrix correspond to the 5 branches of the spanning tree, and the first 3 columns forming C_c correspond to the chords.

$$C = \left[c_{ij}\right]_{5\times 8} = [C_c | I_5]$$

$$\begin{array}{c c} & \begin{array}{ccc|ccccc} \multicolumn{3}{c|}{\text{Chords}} & \multicolumn{5}{c}{\text{Branches}} \\ b & c & d & a & e & f & g & h \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \left[\begin{array}{ccc|ccccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \end{array}$$

Some Application of Fundamental Cutset Matrix:

Problem:
A company has 5 servers connected as follows: (A–B), (B–C), (C–D), (D–E), (A–E), (B–D)

Tasks:

→ Compute the rank of the graph.

→ Construct a fundamental cut-set matrix using a spanning tree.

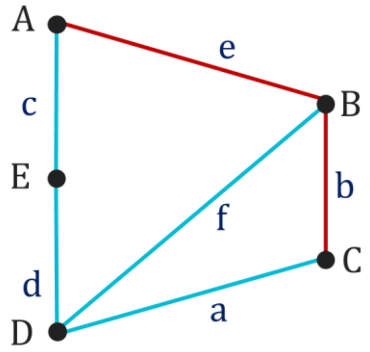
→ Identify the minimum link failures that disconnect the network.

Solution:

→ First we draw graph from given instruction.

→ We have given that: A company has 5 servers connected as follows:

$(\mathbf{A-B}),\ (\mathbf{B-C}),\ (\mathbf{C-D}),\ (\mathbf{D-E}),\ (\mathbf{A-E}),\ (\mathbf{B-D})$



→ Consider spanning tree of following graph (blue lines).

→ Now, we find all of its fundamental cut sets corresponding to all of its branch.

→ Here, graph have 4 fundamental cut set and 6 edges. As graph have 4 branches and 2 chord.

→ That means we get 4×6 fundamental cut-set matrix of given graph.

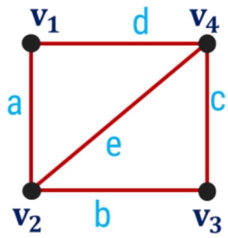
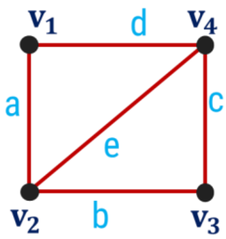
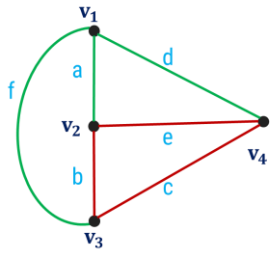
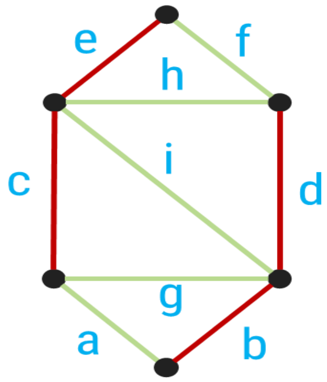
→ Hence, in fundamental cutset matrix the last 4 columns forming the identity matrix correspond to the 4 branches of the spanning tree, and the first 2 columns forming C_c correspond to the chords.

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cc|cccc} b & e & c & a & f & d \end{array} \\ \left[\begin{array}{cc|cccc} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \end{array}\right] \end{array}$$

→ So, in fundamental cut set matrix we have row with two 1's which is the minimum that means 2 edges (for e.g. e, c) is the minimum link failures that disconnect the network.

→ Also from fundamental cutset matrix it is clear that rank of graph is 4.

Example of Method-2: Cut-set Matrix and it's properties

C	1	Find the cut-set matrix for the following graph.	
C	2	Find Fundamental Cut-Set Matrix For Following Graph	
C	3	Find the Fundamental Cut-Set Matrix For Following Graph with respect to given spanning tree (green lines).	
C	4	A network of 6 servers has edges: (A–B), (B–C), (C–D), (D–E), (E–F), (A–F), (B–E). Tasks: 1. Compute rank. 2. Construct a fundamental cut-set matrix using a spanning tree. 3. Identify the minimum link failures that disconnect the network.	
H	5	Find the fundamental cutset matrix for $\mathbf{K_5}$.	
H	6	Find the fundamental cutset matrix of $\mathbf{S_5}$.	
H	7	Find the fundamental cutset matrix of $\mathbf{C_5}$.	
H	8	Find the fundamental cutset matrix of the following graph. 	

Method – 3 ⇝ Eigen Values and Eigen Vector

Eigen Values and Eigen Vectors

→ Let A be an $n \times n$ matrix, then the scalar λ is known as eigen value of A, if there exists a non-zero vector X such that $AX = \lambda X$.

→ The non-zero vector X is known as eigen vector of A corresponding to eigen value λ.

Characteristic Equation

→ Let A be a square matrix of order n and I be an identity matrix of order n. Then $|\mathbf{A} - \boldsymbol{\lambda}\mathbf{I}| = \mathbf{0}$ is known as characteristic equation, where λ is a scalar.

→ The characteristic equation of matrix A of order 2×2 is $\boldsymbol{\lambda^2 - S_1\lambda + S_2 = 0}$ where $S_1 = tr(A)$ and $S_2 = |A|$

→ The characteristic equation of matrix A of order 3×3 is $\boldsymbol{\lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = 0}$ where $S_1 = tr(A)$, $S_2 =$ sum of minors of principal diagonal elements and $S_3 = |A|$

Remarks

→ Let A be a square matrix of order n, then

- A n eigen value of A is a scalar λ such that $|A - \lambda I| = 0$.
- The eigen vectors of A corresponding to eigen value λ are the non-zero solutions of the system $(A - \lambda I) \cdot X = O$.

→ Eigen value is also known as characteristic root/latent value/proper roots and eigen vector is known as characteristic vector/latent vector/proper vector corresponding to the eigen value λ of the matrix.

→ The set of all eigenvalues of matrix A is called Spectrum of A.

Properties of Eigen Value and Eigen Vector

→ $Trace(A) =$ Sum of all the eigen values of matrix A

→ $Det(A) =$ Product of all the eigen values of matrix A

→ If one of the eigen value of matrix A is zero, then $|A| = 0$, hence A^{-1} does not exist.

→ The eigen values of triangular matrix are the elements on its principal diagonal.

→ The square matrix A and A^T have the same eigen values but eigen vectors need not to be same.

→ If λ is an eigen value of a non-singular matrix A and X is an eigen vector correspond to λ, then

- Eigen value of A^{-1} is $\frac{1}{\lambda}$ and X is corresponding eigen vector.

- Eigen value of A^k is λ^k and X is corresponding eigen vector; $k \in \mathbb{R}$
- Eigen value of $A \pm kI$ is $\lambda \pm k$; $k \in \mathbb{R}$
- Eigen value of kA is $k\lambda$; $k \in \mathbb{R}$

$\rightarrow$ **Procedure to find the eigen values, eigen vectors for a matrix A of order 3×3**

- Write the characteristic equation $\lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = 0$ and find S_1, S_2 and S_3.
- Find the roots of the characteristic equation. These are the Eigen Values of A, say $\lambda_1, \lambda_2, \lambda_3$.
- Solve the homogeneous system $(A - \lambda I) \cdot X = O$ for each eigen value by using Gauss Elimination Method.
- Eigen vector is the solution X of above system.

$\rightarrow$ The procedure remains same for the matrices of order 2.

Remarks:

A matrix is invertible if its inverse exists.

Example of Method-3: Eigen Values and Eigen Vector

C	1	Find the eigen values and eigen vectors of the matrix $A = \begin{bmatrix} 3 & 1 & 4 \\ 0 & 2 & 6 \\ 0 & 0 & 5 \end{bmatrix}$. **Answer:** $\boldsymbol{\lambda = 2 \rightsquigarrow X = [-1 \quad 1 \quad 0]^T, \quad \lambda = 3 \rightsquigarrow X = [1 \quad 0 \quad 0]^T}$ $\boldsymbol{\lambda = 5 \rightsquigarrow X = [3 \quad 2 \quad 1]^T}$
C	2	If $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, then find the eigen values and eigen vectors corresponding to each eigen value of A. Also, write the eigen space for each eigen values. **Answer:** $\boldsymbol{\lambda = -1 \rightsquigarrow X = [-1 \quad 1]^T, \quad \lambda = 1 \rightsquigarrow X = [1 \quad 1]^T}$
C	3	Find the adjacency eigen values and eigen vector for complete graph $\mathbf{K_4}$. **Answer:** $\boldsymbol{\lambda = -1, -1, -1, 3.}$ & **Eigen Vector** $= [-3 \quad 1 \quad 1 \quad 1]^T$ **corresponding to** -1 & $= [1 \quad 1 \quad 1 \quad 1]^T$ **corresponding to 3.**
H	4	Find the eigen values of $A = \begin{bmatrix} -5 & 4 & 34 \\ 0 & 0 & 4 \\ 0 & 0 & 4 \end{bmatrix}$. Is it invertible? **Answer:** $-5, \ 0, \ 4$ & **No**
H	5	Find the eigen values of the matrix $A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$. **Answer:** $\boldsymbol{\lambda = -1, \ -1,}$ **and 2**
H	6	Find the Laplacian eigen values and eigen vector for complete graph $\mathbf{K_4}$. **Answer:** $\boldsymbol{\lambda = -1, \ -1,}$ **and 2**
H	7	Find the Laplacian and adjacency eigen value of P_4 and S_4. **Answer:** $\boldsymbol{\lambda = -1, \ -1,}$ **and 2**

Method – 4 ⇝ Visualization using Eigen vector

Spectral Clustering:

→ There are three main types of clustering:

(1) Bottom-Up, (2) Assignment-Based, and (3) Top-Down.

→ The bottom-up variety was like the hierarchical agglomerative clustering where we start with very small clusters and build bigger clusters.

→ The assignment based clustering was like the k-center or the k-means variety were we "assign" each object to a center.

→ The third type, top-down clustering, is what we will be discussing here. It starts from one big cluster and gradually divides the big clusters into smaller and smaller clusters.

→ Find the best cut of the data into two pieces.

→ Recur on both pieces until that data should not be split anymore.

→ So how to cluster a graph? A cluster is a subset $S \subset V$.

→ We are performing top down clustering, so we only need to consider a subset S and its compliment $\bar{S} = V - S$.

→ In general, we want many edges within a cluster (small width), and few edges between clusters (large split).

→ The volume of a cluster is $\mathrm{Vol}(\mathbf{S})$ = the number of edges with at least one vertex in $\mathbf{V}$.

→ The cut between two clusters S, T is $\mathrm{Cut}(\mathbf{S}, \mathbf{T})$ = the number of edges with one vertex in **S** and the other in **T**.

→ Then we want a large $\mathrm{Vol}(S)$ for each cluster and a small $\mathrm{Cut}(\mathbf{S}, \mathbf{T})$ for each pair of clusters.

Steps for Spectral Clustering with normalized Laplacian matrix:

- Start with the Laplacian matrix and find the eigenvector of a matrix.
- There are several eigenvectors of L (the normalized Laplacian): list them sorted by $\boldsymbol{\lambda}$(smaller to larger).
- This can be calculated easily in python using the eigvals, V = np.linalg.eigh(L) command.
- The first eigenvalue of the Laplacian is always 0, up to numerical error.

- The second eigenvector of the normalized Laplacian is a very important descriptor of a graph.
    - It tells us how to best cut the graph.
    - It tells us how “best” to put all of the vertices on a single line. It is called the **Fiedler vector.**
- We can set cluster $S = \{v_i \in V : u_2(v_i) < 0\}$ and cluster $T = V - S$.

More about Spectral Clustering:

→ Alternatively, we can use the first d-eigenvectors (scaled by eigenvalues) to embed the vertices in R^d .

→ Then we can use any Euclidean clustering algorithm (such as k-means clustering).

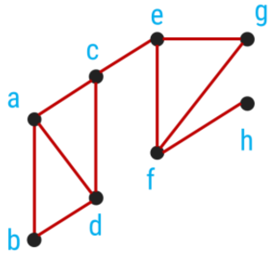
→ More generally, the adjacency matrix need not be $0-1$.

→ It can be filled with the similarity value defined by some similarity between element; then A stands for affinity.

→ The diagonal is defined as the sum of elements in a row (or column — it must be symmetric). Then spectral clustering can be run as before.

→ When the similarity of a pair is very small, it is a good heuristic to round the values down to 0 in the matrix to make the algorithm run faster.

Example of Method-4: Perfect Matching and Hall's Theorem (without proof)

C	1	**Find 2 cluster using spectral clustering of following graph.**  **Answer**: $\mathbf{S = ['a', 'b', 'c', 'd']}$ **and** $\mathbf{T = ['e', 'f', 'g', 'h']}$.
H	2	**Find 2 cluster using spectral clustering of following graph.** Graph vertices: a, b, c, d, e, f, g. Edges: (a,b), (b,c), (c,d), (d,a), (a,c), (e,f), (f,g), (e,g), (c,e), (b,e). **Answer**: $\mathbf{S = ['a', 'b', 'c', 'd']}$ **and** $\mathbf{T = ['e', 'f', 'g']}$.

* * * * * **End of the Unit** * * * * *