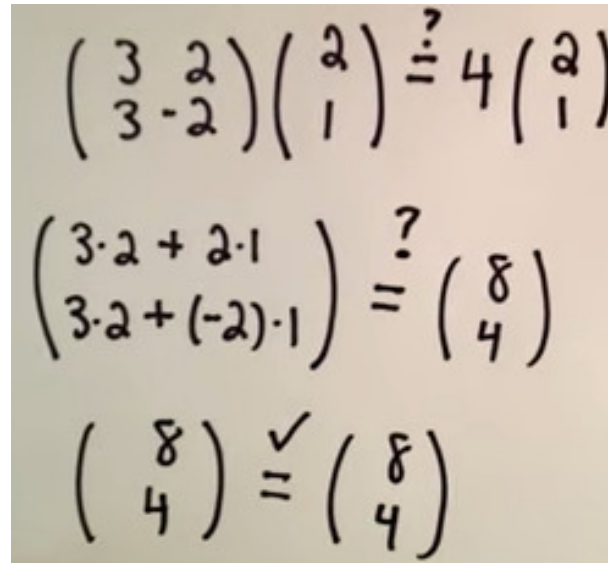# Spectral Analysis

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Eigenvalue and Eigenvector

- Let A be an nxn matrix.
- A scalar λ is called an Eigenvalue of A if there is a non-zero vector X such that AX = λX. Such a vector X is called an Eigenvector of A corresponding to λ.
- Example: $\begin{bmatrix} 2 \\ 1 \end{bmatrix}$ is an Eigenvector of A = $\begin{bmatrix} 3 & 2 \\ 3 & -2 \end{bmatrix}$ for λ = 4

$$\begin{pmatrix} 3 & 2 \\ 3 & -2 \end{pmatrix}\begin{pmatrix} 2 \\ 1 \end{pmatrix} \overset{?}{=} 4\begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 3\cdot 2 + 2\cdot 1 \\ 3\cdot 2 + (-2)\cdot 1 \end{pmatrix} \overset{?}{=} \begin{pmatrix} 8 \\ 4 \end{pmatrix}$$

$$\begin{pmatrix} 8 \\ 4 \end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} 8 \\ 4 \end{pmatrix}$$

Finding Eigenvalues and Eigenvectors

$A = \begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix}$

① $\lambda I = \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$

② $A - \lambda I = \begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$

$= \begin{bmatrix} 7-\lambda & 3 \\ 3 & -1-\lambda \end{bmatrix}$

③ $\det \begin{bmatrix} 7-\lambda & 3 \\ 3 & -1-\lambda \end{bmatrix}$

$= (7-\lambda)(-1-\lambda) - (3)(3)$

$= -7 - 7\lambda + \lambda + \lambda^2 - 9$

$= \lambda^2 - 6\lambda - 16$

(4) Solving for λ:
(λ – 8) (λ + 2) = 0
λ = 8 and λ = -2 are the Eigen values

(5) Consider A – λ I

⑤ $\begin{bmatrix} 7-\lambda & 3 \\ 3 & -1-\lambda \end{bmatrix}$

$\lambda = 8$:

$\begin{bmatrix} 7-8 & 3 \\ 3 & -1-8 \end{bmatrix} = \begin{bmatrix} -1 & 3 \\ 3 & -9 \end{bmatrix}$ = B

Solve B X = 0

$\begin{pmatrix} -1 & 3 \\ 3 & -9 \end{pmatrix} \begin{pmatrix} X1 \\ X2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

-X1 + 3X2 = 0 → X1 = 3X2
3X1 – 9X2 = 0 → 3X1 = 9X2 ➔ X1 = 3X2

If X2 = 1; $\begin{bmatrix} 3 \\ 1 \end{bmatrix}$ is an eigenvector
X1 = 3   for λ = 8

Finding Eigenvalues and Eigenvectors

For $\lambda = -2$

$$\begin{bmatrix} 7-(-2) & 3 \\ 3 & -1-(-2) \end{bmatrix} = \begin{bmatrix} 9 & 3 \\ 3 & 1 \end{bmatrix}$$

Solve B X = 0

$$\begin{bmatrix} 9 & 3 \\ 3 & 1 \end{bmatrix}\begin{bmatrix} X1 \\ X2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$9X1 + 3X2 = 0 \longrightarrow X2 = -3X1$

$3X1 + X2 = 0 \longrightarrow X2 = -3X1$

If X1 = 1; $\begin{bmatrix} 1 \\ -3 \end{bmatrix}$ is an eigenvector

X2 = -3   for **λ = -2**

Verification $A = \begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix}$

AX = λX

For $\lambda = 8$ and $X = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$

$$\begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix}\begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 24 \\ 8 \end{bmatrix} = 8\begin{bmatrix} 3 \\ 1 \end{bmatrix}$$

An *n*x*n* matrix has *n* eigenvalues and the corresponding eigenvectors.

Spectral Analysis

- Spectral decomposition is a method of projecting the characteristics of a network graph in n-dimensions or directions (that are mutually perpendicular) where n is the number of vertices in the graph.

- The projection in each direction is represented in the form of a scalar value (called the eigenvalue) and its corresponding vector with entries for each vertex (called the eigenvector).

- The largest eigenvalue of the projection is called the principal eigenvalue (a.k.a. spectral radius) and the corresponding eigenvector is called the principal eigenvector.

- We will use the adjacency matrix of a network graph to determine its eigenvalues and eigenvectors.

Example: Eigenvalues and Eigenvectors

Edge list:
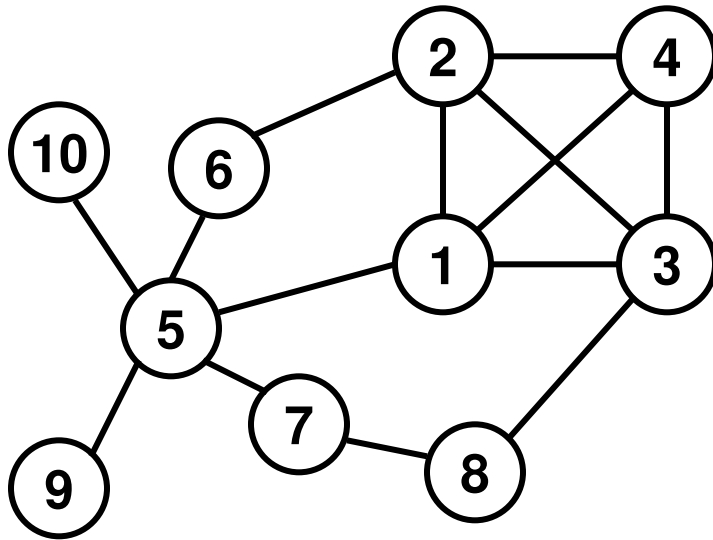
1	2
1	3
1	4
1	5
2	3
2	4
2	6
3	4
3	8
5	6
5	7
5	9
5	10
7	8

List of edges written in the increasing order of the node IDs from left to right and top to bottom.

Property: For a matrix with all positive entries, the Principal Eigenvalue is always positive & the entries in the Principal Eigenvector are also positive

Node IDs ← **Eigenvalues** →

|	3.3893	1.888	1.1131	0.3197	0	-0.3741	-0.8564	-1.3098	-1.6828	-2.4871
1	0.4741	0.0641	-0.1261	0.2899	0	-0.3898	0.5219	-0.0776	0.3210	0.3711
2	0.4568	0.2043	-0.2089	-0.3262	0	0.0872	-0.2158	-0.6614	0.1384	-0.2979
3	0.4453	0.2648	0.2600	0.1054	0	0.3619	0.2312	0.0638	-0.6797	0.0477
4	0.4060	0.2824	-0.0674	0.2161	0	-0.1585	-0.6275	0.5155	0.1309	-0.0486
5	0.2986	-0.6305	-0.1241	0.0974	0	-0.1448	0.1651	0.1838	-0.1298	-0.6242
6	0.2229	-0.2257	-0.2991	-0.7157	0	0.1538	0.0591	0.3646	-0.0051	0.3708
7	0.1390	-0.3609	0.5100	-0.1521	0	-0.4838	-0.3369	-0.2471	-0.2518	0.3086
8	0.1724	-0.0509	0.6917	-0.1460	0	0.3258	0.1234	0.1399	0.5536	-0.1433
9	0.0881	-0.3339	-0.1114	0.3046	-0.7071	0.3870	-0.1928	-0.1403	0.0771	0.2510
10	0.0881	-0.3339	-0.1114	0.3046	0.7071	0.3870	-0.1928	-0.1403	0.0771	0.2510

Each column corresponds to an Eigenvector with an entry for each node

Spectral Radius Ratio for Node Degree

- Spectral radius ratio for node degree (for an undirected graph) is the ratio of the principal eigenvalue of the adjacency matrix and the average degree of the vertices in the graph.
- If Kmin, Kavg and Kmax are the minimum, average and maximum values for the node degrees, then:
  - Kmin ≤ Kavg ≤ Principal Eigenvalue ≤ Kmax
- So, the spectral radius ratio for node degree of a graph is always greater than or equal to 1.

- The spectral radius ratio for node degree is a measure of the variation in the node degrees. The farther is the value from 1, the larger the variation in node degree.

- The spectral radius ratio for node degree can be uniformly applied across networks of all size and be used to evaluate the relative variation in node degree.

Spectral Radius Ratio for Node Degree
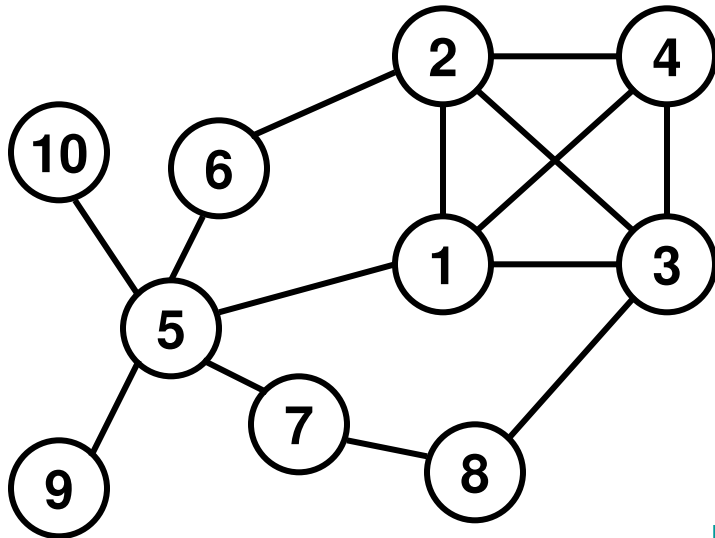
Avg. Degree = Sum of Node Degrees / N
= (4 + 4 + 4 + 3 + 5 + 2 + 2 + 2 + 1 + 1)/10
= 2.8

Principal Eigenvalue = 3.3893
Spectral Radius Ratio for Node Degree
= 3.3893 / 2.8 = 1.21
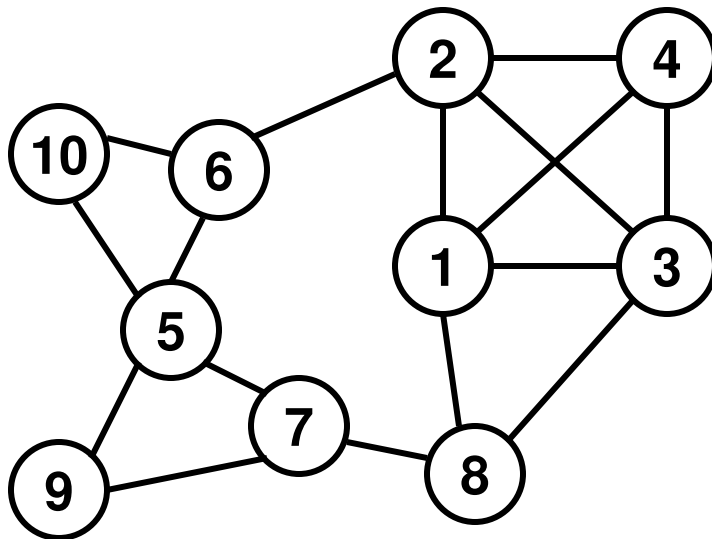
1	2
1	3
1	4
1	8
2	3
2	4
2	6
3	4
3	8
5	6
5	7
5	9
5	10
6	10
7	8
7	9

Avg. Degree = Sum of Node Degrees / N
= (4 + 4 + 4 + 3 + 4 + 3 + 3 + 3 + 2 + 2)/10
= 3.2

Principal Eigenvalue = 3.4735
Spectral Radius Ratio for Node Degree
= 3.4735 / 3.2 = 1.09

Applications

- Bipartivity Index: Detection of bipartivity in graphs
- Estrada Index: Protein folding
- Laplacian Matrix: Determining the number of components, connectivity and number of spanning trees in a graph
- Hierarchical Community Detection
- Prediction of Graph Isomorphism

Eigen Values of a Bipartite Network

- There are even number of vertices.
- Let λ1, λ2, λ3, …, λn be the n Eigenvalues of an n-node network.
- For any j = 1, 2, …, n/2, if $\lambda_j = | - \lambda_{n-j+1}|$, then the network is almost bi-partite.
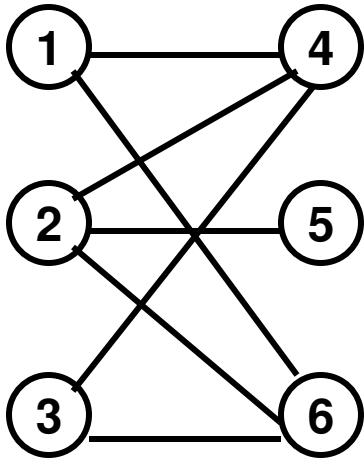
0	0	0	1	0	1
0	0	0	1	1	1
0	0	0	1	0	1
1	1	1	0	0	0
0	1	0	0	0	0
1	1	1	0	0	0

Eigenvalues
-2.5243
-0.7923
0
0
0.7923
2.5243

Bipartivity Check

- A bi-partite graph is the one that has two partitions V1 and V2 of its vertices such that
  - V1 U V2 = V; V1 n V2 = Φ.
  - No edges within V1 and within V2.
  - All edges are those connecting V1 and V2.
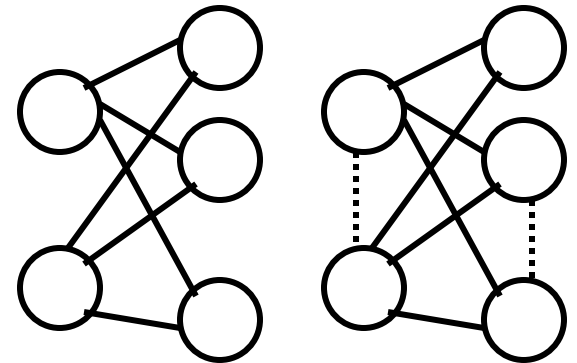
  There should be NO odd length cycles in a truly bi-partite network

- Graphs can be considered close to bi-partite if there are few edges (not a significant number) called the frustrated edges that connect vertices within V1 and/or V2.

Computing the Bipartite Measure

Compute the Eigenvalues (λ1, λ2, λ3, …, λn) of the nxn adjacency matrix.

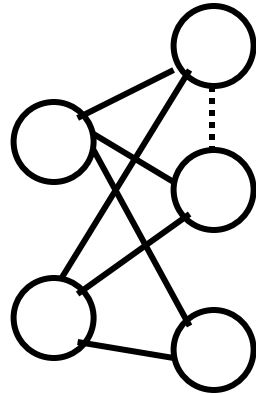$$b_S(G) = \frac{\sum_{j=1}^{n} \cosh(\lambda_j)}{\sum_{j=1}^{n} \cosh(\lambda_j) + \sum_{j=1}^{n} \sinh(\lambda_j)}$$

For a "truly" bi-partite graph, $b_S(G) = 1$; the sinh terms add to 0.

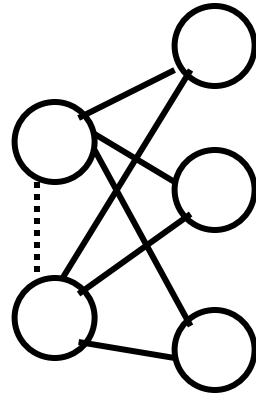**For a "close-to" bi-partite graph, $b_S(G) < 1$; the sinh terms add up to some small positive value.**

Bipartivity Measure: Examples
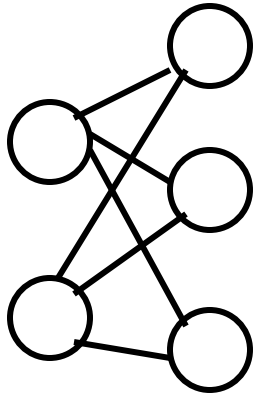
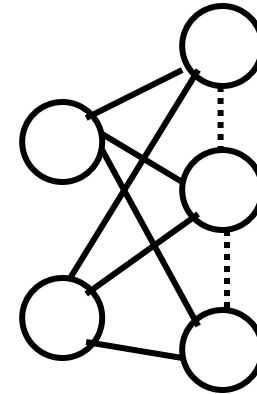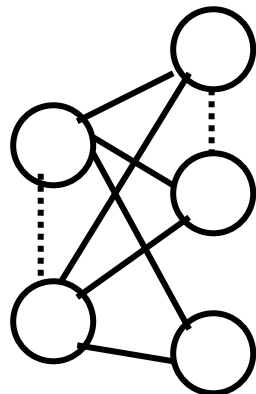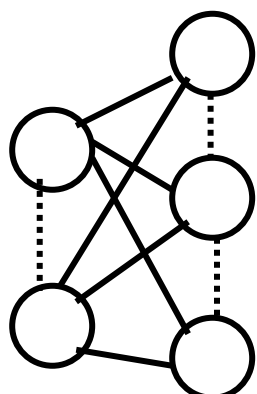

$b_S(G) = 1.0$　　$b_S(G) = 0.829$　　$b_S(G) = 0.769$　　$b_S(G) = 0.731$
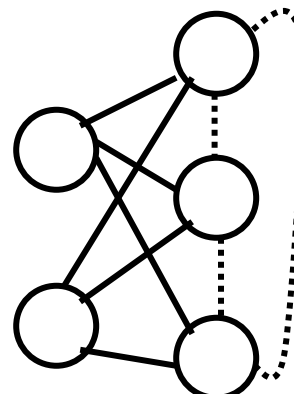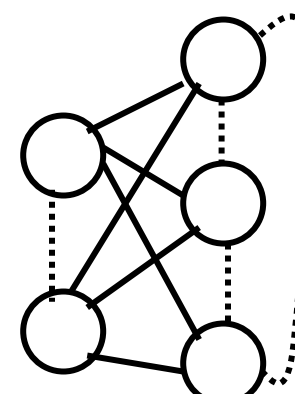
$b_S(G) = 0.692$　　$b_S(G) = 0.645$　　$b_S(G) = 0.645$　　$b_S(G) = 0.597$

For a given number of frustrated links, a larger bipartivity measure is observed if more of the frustrated links are present in the network with the larger subset.

Bipartivity of Real Networks

Type: Information	
Network	**Bipartivity Measure**
SciMet	0.500
Roget	0.529

Type: Social	
Network	**Bipartivity Measure**
Drugs	0.500
Corporate Elite	0.500
Karate Club	0.597
Saw Mill	0.749

Type: Food webs	
Network	**Bipartivity Measure**
Coachella	0.500
El Verde	0.500
Grassland	0.743
Stony stream	0.815

Type: PPIs	
Network	**Bipartivity Measure**
Yeast	0.500
Human	0.576
H. Pylori	0.711
A. Fulgidus	0.976

Type: Transcription	
Network	**Bipartivity Measure**
Urchin	0.618
E. Coli	0.831
Yeast	0.960

Type: Technological	
Network	**Bipartivity Measure**
USAir97	0.500
Internet	0.502
Electronic3	0.952

Identifying Bipartite Subsets using Eigenvalue and Eigenvector

- We identify the smallest Eigenvalue (most likely a negative value), hereafter called the bi-partite Eigenvalue, and its corresponding Eigenvector, hereafter called the bi-partite Eigenvector.

- The values in the bi-partite Eigenvector will be positive and negative.

  - The node IDs whose entries are of the same sign in the bi-partite Eigenvector form the two subsets.

    - The vertices that are of the same sign are more likely not to have links between them, and are more likely to have links with vertices of the other sign.

  - Each of the two subsets will have the minimum (or zero, if possible) number of frustrated links. Most of the links are likely to be between the vertices in the two subsets.

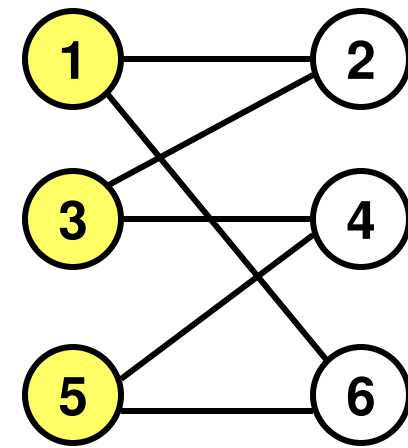# Identifying Bipartite Subsets using Eigenvalue and Eigenvector: Ex. 1 (1)
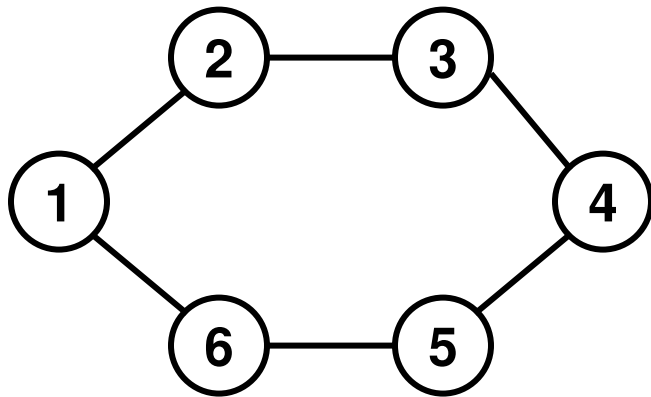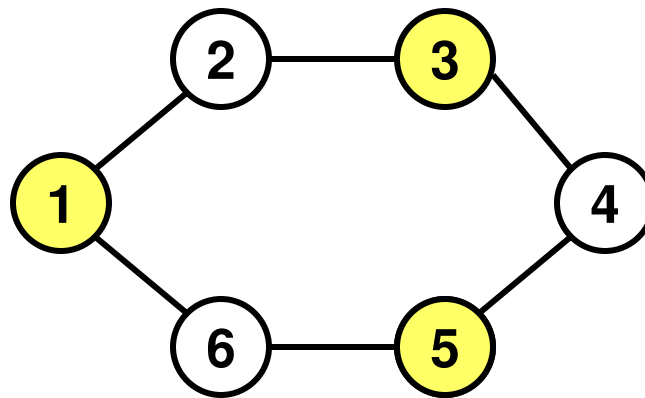
Identifying Bipartite Subsets using Eigenvalue and Eigenvector: Ex. 1 (2)

Eigenvalue, λ	cosh(λ)	sinh(λ)
-2	3.7622	-3.6269
-1	1.5431	-1.1752
-1	1.5431	-1.1752
1	1.5431	1.1752
1	1.5431	1.1752
2	3.7622	-3.6269
----------	----------	----------
Total	13.6968	0

$$b_S(G) = \frac{\sum_{j=1}^{n} \cosh(\lambda_j)}{\sum_{j=1}^{n} \cosh(\lambda_j) + \sum_{j=1}^{n} \sinh(\lambda_j)}$$

$$b_S(G) = \frac{13.6968}{(13.6968 + 0)}$$

$$= 1.0$$

Identifying Bipartite Subsets using Eigenvalue and Eigenvector: Ex. 2 (1)

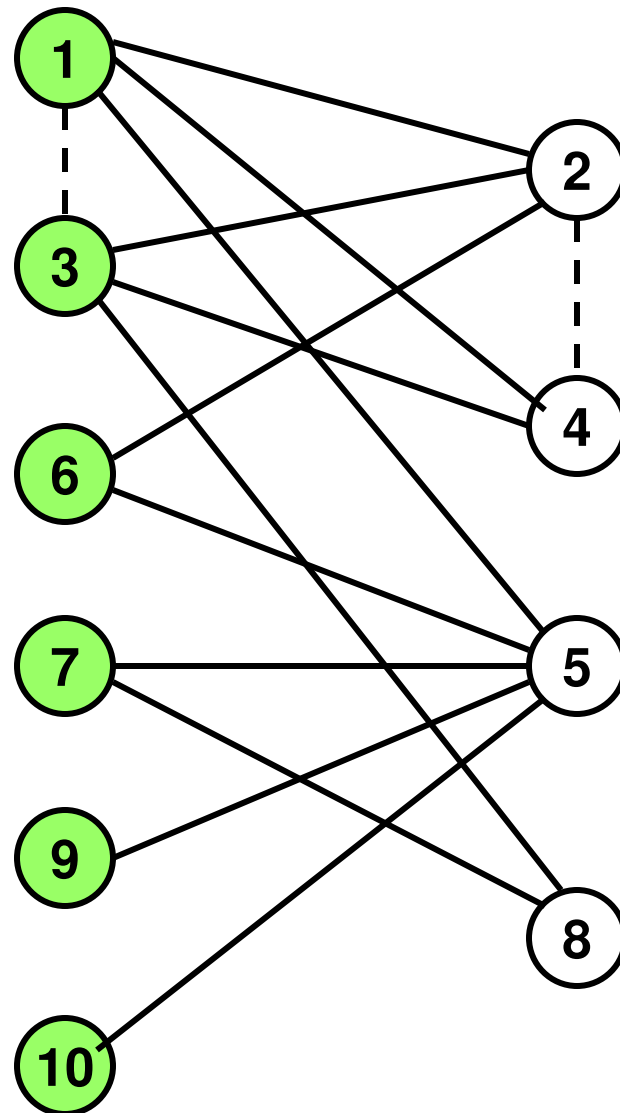# Identifying Bipartite Subsets using Eigenvalue and Eigenvector: Ex. 2 (2)

Based on the lowest Negative Eigenvalue -2.4870836366555165:

1	0.3711379191456978
2	-0.2979483534591263
3	0.04772178019913417
4	-0.048615713642947846
5	-0.6242087587467021
6	0.3707784887547619
7	0.3085825736313854
8	-0.14326191068896146
9	0.25098020410206323
10	0.250980204102063

Identifying Bipartite Subsets using Eigenvalue and Eigenvector: Ex. 2 (3)

| Eigenvalue, λ	cosh(λ)	sinh(λ)
-2.4871	6.0547	-5.9716
-1.6828	2.7832	-2.5974
-1.3098	1.9877	-1.7178
-0.8564	1.3897	-0.9650
-0.3741	1.0708	-0.3829
0	1.0	0
0.3197	1.0515	0.3252
1.1131	1.6862	1.3576
1.8880	3.3788	3.2274
3.3893	14.839	14.8057

Total	35.2416	8.0812

$$b_S(G) = \frac{\sum_{j=1}^{n} \cosh(\lambda_j)}{\sum_{j=1}^{n} \cosh(\lambda_j) + \sum_{j=1}^{n} \sinh(\lambda_j)}$$

$$b_S(G) = \frac{35.2416}{(35.2416 + 8.0812)}$$

$$= 0.8135$$

Bipartite Partition Detection: Digraph

- When confronted with a directed graph, first transform the directed graph to an undirected graph and determine the two partitions as explained previously using the Eigenvector approach.

- After identifying the partitions, restore the directions of the edges.

- In a directed graph, the edges typically point from one set of vertices to the other set of vertices.
  - There could be scenarios where the edges could point in the reverse direction; as long as we know the direction of the edges, we could restore them after determining the two partitions.
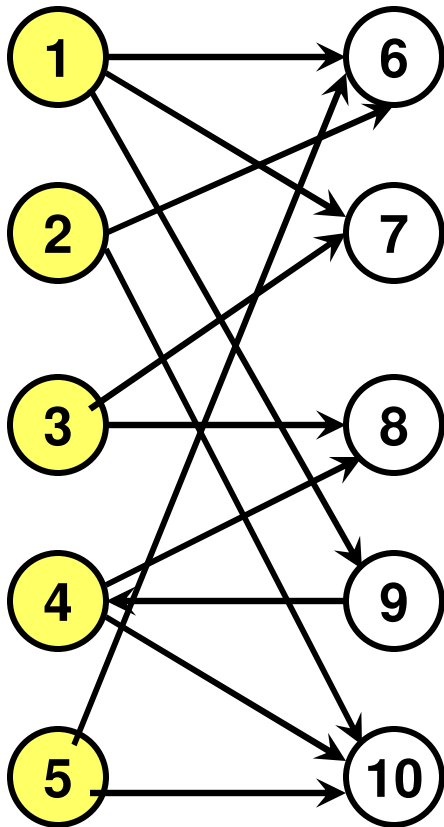
Digraph Bipartivity Detection: Example (1)

Edge list:
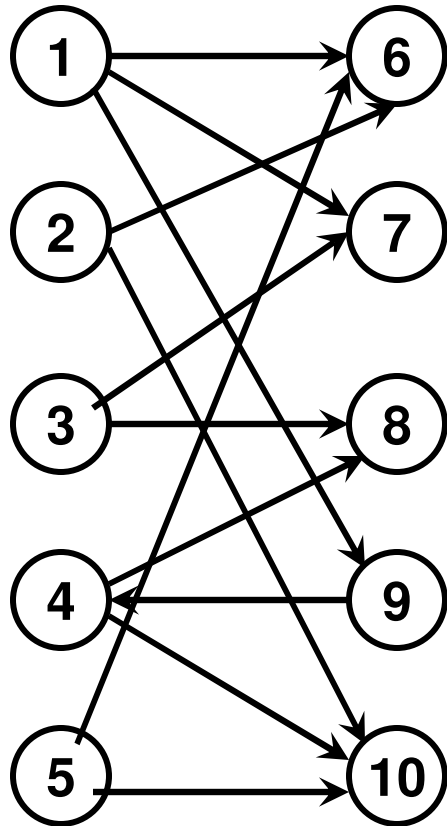
1	6
1	7
1	9
2	6
2	10
3	7
3	8
4	8
4	10
5	6
5	10

Adjacency matrix:

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	1	1	0	1	0
2	0	0	0	0	0	1	0	0	0	1
3	0	0	0	0	0	0	1	1	0	0
4	0	0	0	0	0	0	0	1	0	1
5	0	0	0	0	0	1	0	0	0	1
6	1	1	0	0	1	0	0	0	0	0
7	1	0	1	0	0	0	0	0	0	0
8	0	0	1	1	0	0	0	0	0	0
9	1	0	0	1	0	0	0	0	0	0
10	0	1	0	1	1	0	0	0	0	0

Digraph Bipartivity Detection: Example (2)

Based on the lowest Negative
Eigenvalue -2.3692:
1   -0.352125235 8695437
2   -0.376130057 0544691
3   -0.167935975 2033227
4   -0.254671723 7086407
5   -0.376130057 054469
6   0.466136289 99636475
7   0.219506174 63844993
8   0.178373232 58458782
9   0.148624165 52838364
10 0.425003347 9425025

Protein Folding

- Protein folding is the process by which a protein transforms from a random coil (sequence of amino acids: linear polypeptide chain) to its characteristic 3-dimensional structure that is essential to its expected function.

- The correct three-dimensional structure is essential to function, although some parts of functional proteins may remain unfolded.

- Failure to fold into native structure generally produces inactive proteins, but in some instances misfolded proteins have modified or toxic functionality.

- When modeled as a graph, the more flat (linear chain) is the graph, the less the folding and vice-versa.
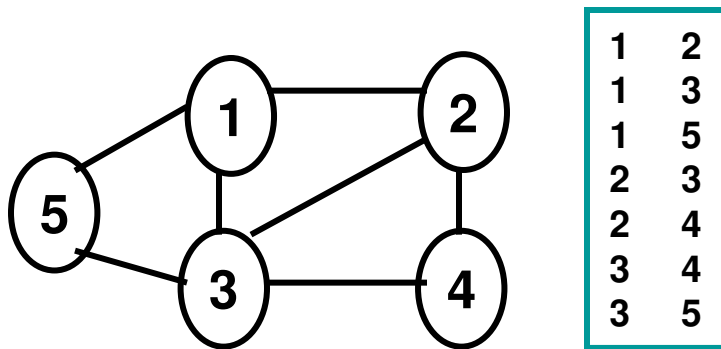
Estrada, E. (2000). "Characterization of 3D molecular structure". *Chem. Phys. Lett.* **(319): 713**

Source: Wikipedia
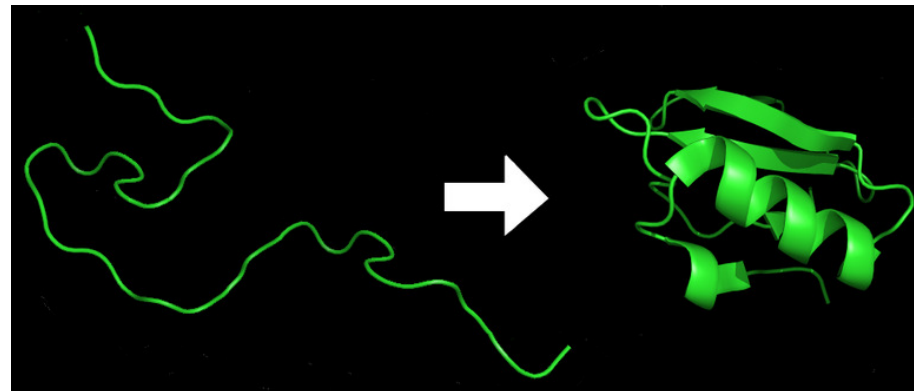
Estrada Index of Graphs

- The Estrada Index can be used to determine the degree of folding of a protein.
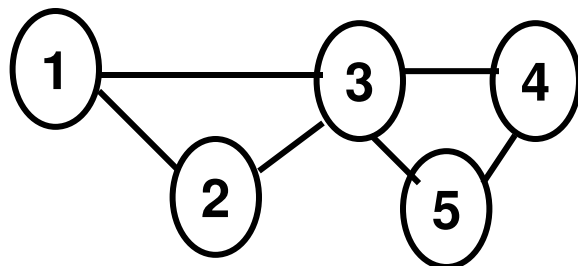 - Larger the Estrada Index, the larger the folding.

$e^{\lambda j}$

1	2
1	3
1	5
2	3
2	4
3	4
3	5

$$A = \begin{vmatrix} 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{vmatrix}$$

$\lambda 1 = -1.618$ 0.2
$\lambda 2 = -1.473$ 0.23
$\lambda 3 = -0.463$ 0.63
$\lambda 4 = 0.618$ 1.852
$\lambda 5 = 2.935$ 18.654

$$EE(G) = \sum_{j=1}^{n} e^{\lambda_j}$$

EE(G) = 21.56

$e^{\lambda j}$

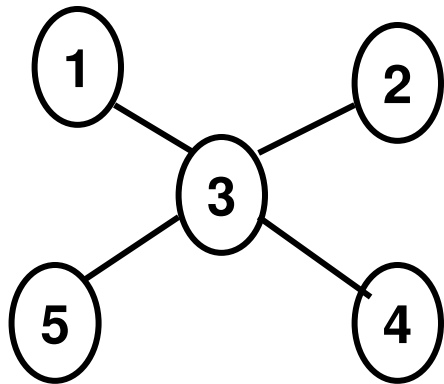| 1	2
1	3
2	3
3	4
3	5
4	5

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

$\lambda 1 = -1.5616$ 0.211
$\lambda 2 = -1$ 0.369
$\lambda 3 = -1$ 0.369
$\lambda 4 = 1$ 2.71
$\lambda 5 = 2.5616$ 12.856

EE(G) = 16.51

Estrada Index of Star and Chain
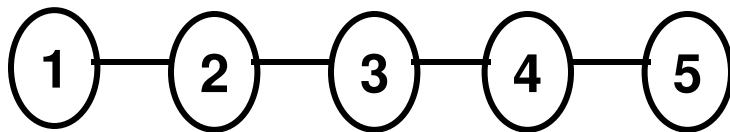

$$EE(G) = \sum_{j=1}^{n} e^{\lambda_j}$$

Star graph:

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

edge list:
1	3
2	3
3	4
3	5

	e^{λ_j}
$\lambda_1 = -2$	0.136
$\lambda_2 = 0$	1
$\lambda_3 = 0$	1
$\lambda_4 = 0$	1
$\lambda_5 = 2$	7.344

EE(G) = 10.48

Chain graph:

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

edge list:
1	3
2	3
3	4
4	5

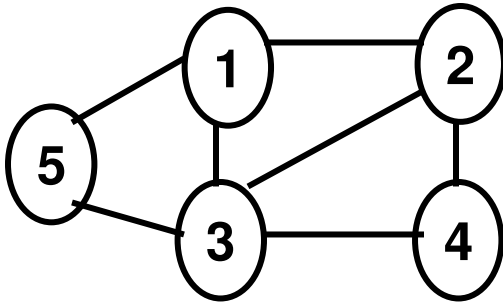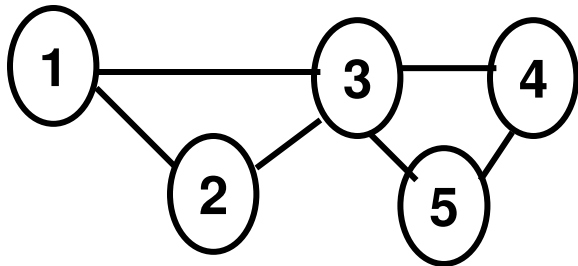|	e^{λ_j}
$\lambda_1 = -1.7321$	0.178
$\lambda_2 = -1$	0.369
$\lambda_3 = 0$	1
$\lambda_4 = 1$	2.71
$\lambda_5 = 1.7321$	5.622

EE(G) = 9.88

Folding Effectiveness

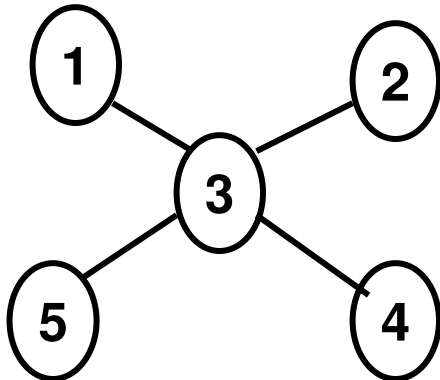$$\text{Folding Effectiveness}(G) = \frac{\text{Estrada Index}(G)}{\text{Estrada Index}(\text{Chain})}$$

Larger and farther the value from 1, the more folded is the protein

Folding Effectiveness (G) = 21.56 / 9.88 = 2.18

**Folding Effectiveness (G) = 16.51 / 9.88 = 1.67**

Folding Effectiveness (G) = 10.48 / 9.88 = 1.06

Components (Clusters)

- The vertices of a graph are said to be in a single component if there is a path between the vertices.
- A graph is said to be connected if all its vertices are in one single component; otherwise, the graph is said to be disconnected and consists of multiple components.
  - Adding one or more links (bridges) can connect the different components
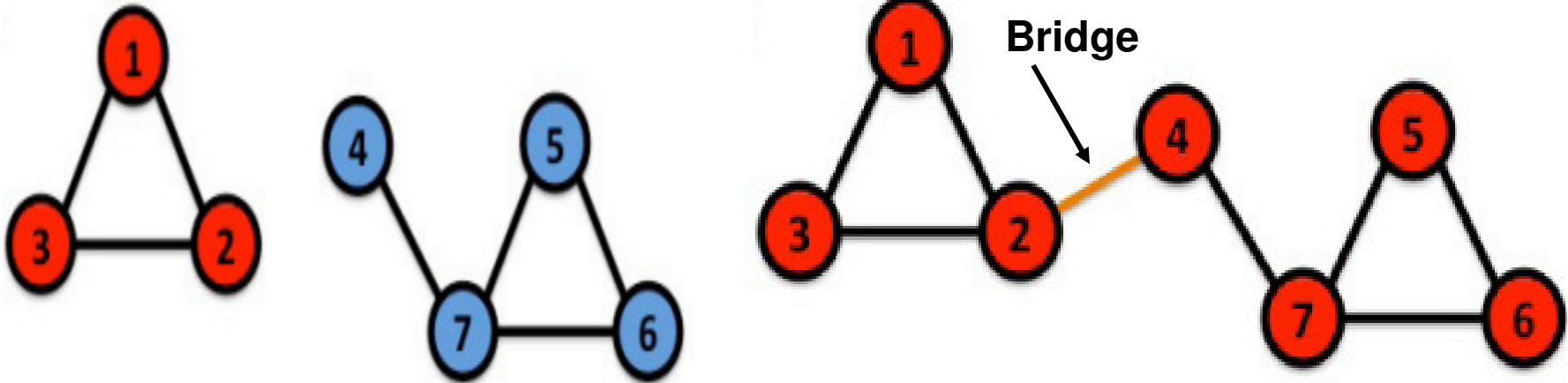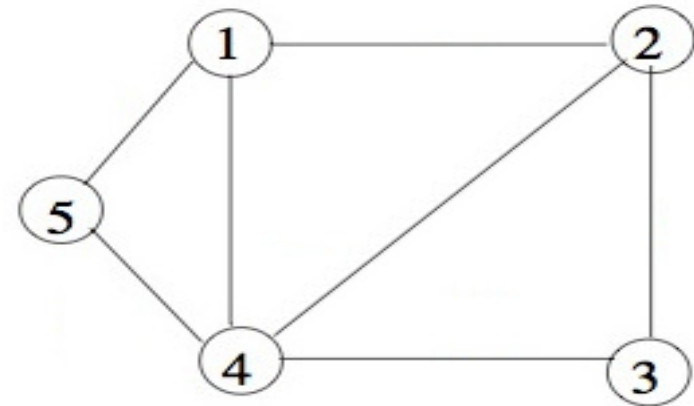
Laplacian Matrix

- Laplacian Matrix L = D – A

$$L_{ij} = \begin{cases} deg(i) & \text{for} \quad i = j \\ -a_{ij} & \text{for} \quad i \neq j \end{cases}$$

$$\begin{pmatrix} 3 & -1 & 0 & -1 & -1 \\ -1 & 3 & -1 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ -1 & -1 & -1 & 4 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

The second smallest eigenvalue of the Laplacian matrix is a measure of the Connectivity of the graph and is called (Fiedler Value).

The n eigenvalues of an n x n Laplacian matrix are all positive.
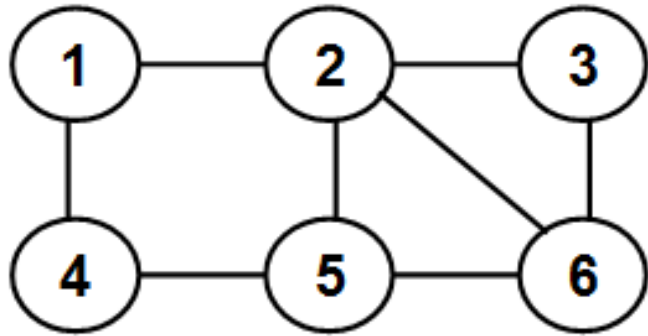
The first eigenvalue is always 0.

The number of 0s among the Eigenvalues of the Laplacian Matrix indicates the number of Connected components of a graph.

The eigenvalues of the above Laplacian matrix are:

0   1.586   3.0   4.414   5.0

Max. Fiedler Value for a graph of n vertices is n (for a complete graph).

Algebraic Connectivity

- The algebraic connectivity of a graph is bounded above by the traditional connectivity of the graph, defined as the minimum number of vertices (a.k.a. articulation points) that need to be removed to disconnect the graph into two or more components.

- However, the traditional connectivity measure (an integer corresponding to the minimum number of vertices to be removed for disconnection) cannot capture the relative strength of the graphs (that have the same number of articulation points).

- For example, if a graph has 2 articulation points, is the graph vulnerable for disconnection due to the removal of any two vertices or some specific two vertices?
  - The algebraic connectivity could be used to quantify the relative strengths of graphs with the same number of articulation points.

Algebraic Connectivity

Laplacian Matrix

	1	2	3	4	5	6
1	2	-1	0	-1	0	0
2	-1	4	-1	0	-1	-1
3	0	-1	2	0	0	-1
4	-1	0	0	2	-1	0
5	0	-1	0	-1	3	-1
6	0	-1	-1	0	-1	3

Eigenvalues

0
1.108
2.295
3.0
4.317
5.278

Graph 1

Algebraic Connectivity: 1.108
Traditional Connectivity: 2

If we remove vertices 1 and 5, Graph 1 will get disconnected, but not Graph 2

Laplacian Matrix

	1	2	3	4	5	6
1	2	-1	0	-1	0	0
2	-1	4	-1	-1	-1	-1
3	0	-1	2	0	0	-1
4	-1	-1	0	2	-1	0
5	0	-1	0	-1	3	-1
6	0	-1	-1	0	-1	3

Eigenvalues

0
1.382
2.382
3.618
4.618
5.999
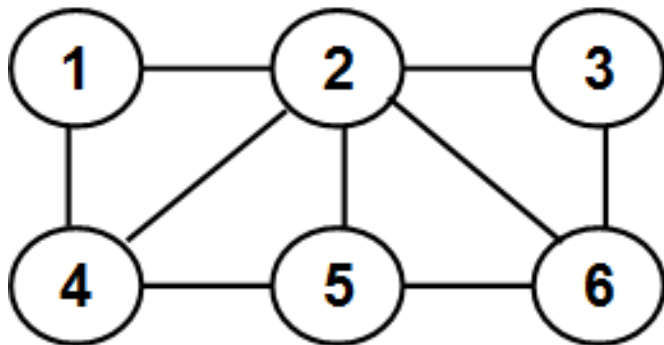
Graph 2

Algebraic Connectivity: 1.382
Traditional Connectivity: 2

Laplacian Matrix
Components

The 7 eigenvalues of the Laplacian Matrix are:

0
0
1.0
3.0
3.0
3.0
4.0
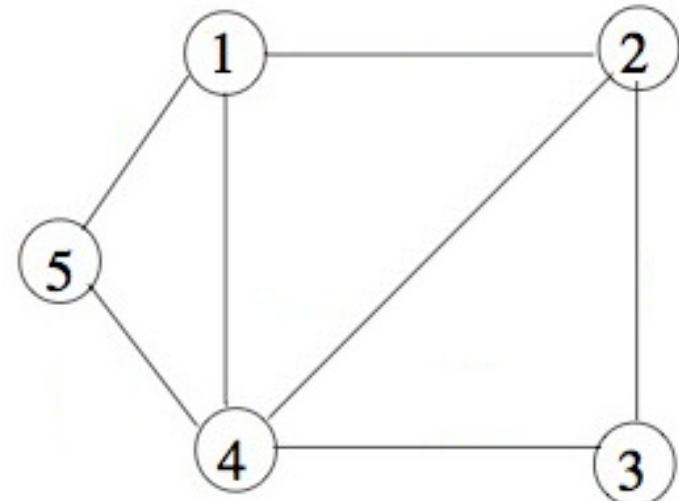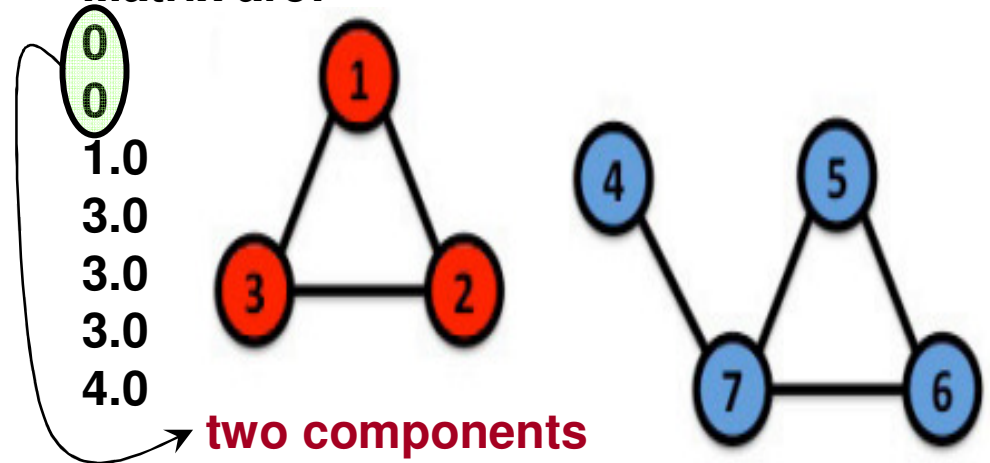
two components

Laplacian Matrix
Spanning Trees

If $\mu_1 = 0 < \mu_2 \leq \mu_3 \leq \ldots \leq \mu_n$ are the n Eigenvalues of the Laplacian matrix of a connected graph of n vertices

The # spanning trees of the graph is then

$$\frac{1}{n} \prod_{i=2}^{n} \mu_i$$

**The five eigenvalues of the Laplacian matrix of the above graph are: 0, 1.586, 3.0, 4.414, 5.0**

# spanning trees = (1/5)(1.586*3*4.414*5) = 21.

Community

- Community: It is formed by individuals such that those within a group <u>interact</u> with each other more frequently than with those outside the group.
- The paths among vertices within a community is most likely to involve only the other vertices within the community.
- For a highly modular community of vertices, the number of edges connecting them within the community is significantly greater than the number of edges connecting them to vertices outside the community.
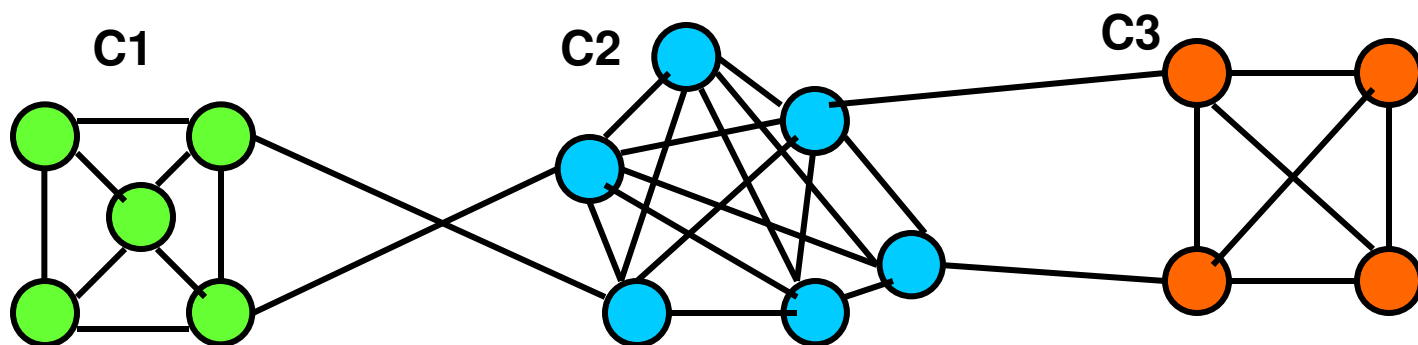
Modularity Maximization

- Modularity measures the strength of a community partition by taking into account the degree distribution.
- Given a network with *m* edges, the probability of an edge between two nodes *i* and *j* with degrees d_i and d_j respectively is $d_i * d_j / 2m$.
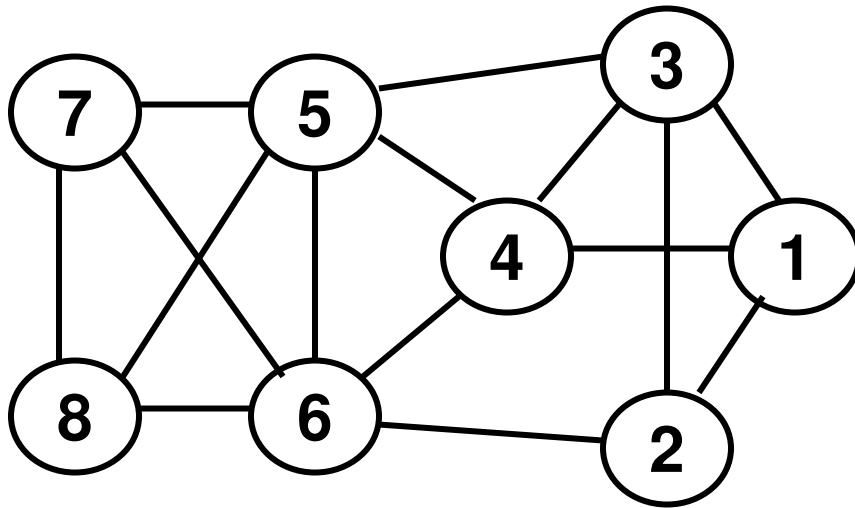
Probability of an edge between nodes 1 and 2 is (3)(3) / (2*15) = 0.30

Strength of a Community, C

$$\sum_{i \in C, j \in C} A_{i,j} - \frac{d_i d_j}{2m}$$

For a network with *k* communities and a total of *m* edges
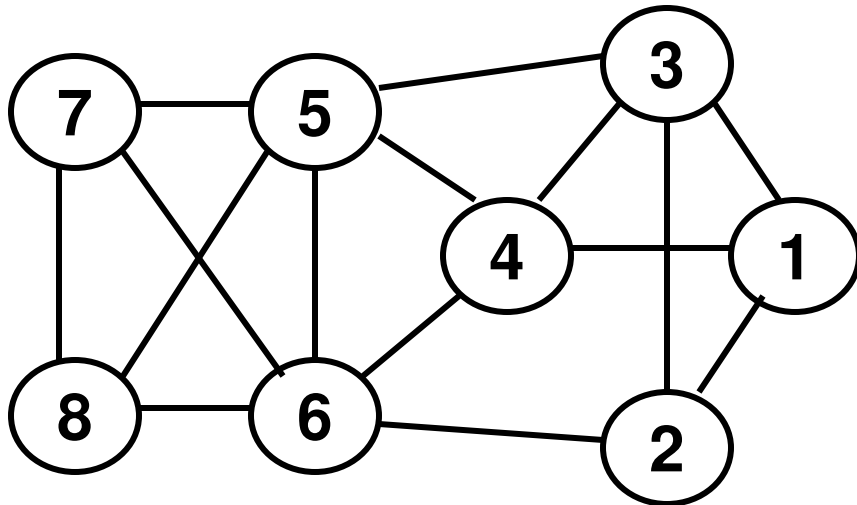
Modularity:

$$Q = \sum_{l=1}^{k} \sum_{i \in C_l, j \in C_l} A_{i,j} - \frac{d_i d_j}{2m}$$

A larger value for Q indicates a good community structure

Modularity Maximization

- The intuition behind the idea of modularity is that a community is a structural element of a network that has been formed in a manner far from a random process.

- If we consider the actual density of links in a community, it should be significantly larger than the density we would expect if the links in the network were formed by a random process.

  – In other words, if two nodes i and j are end up being in the same community, there should be more likely a link between them (i.e., Aij = 1, leading to an overall high value for Q).

  – If i and j end up being in a community such that the chances of having a link between them is just as the same as between any two nodes in the network (i.e., a random network), then the value of Q is more likely to be low (because there could be some Aij = 0 that will bring down the value of Q).

Evaluating Modularity (Example 1)

Community [1, 4, 5, 7]

Edges with Aij = 1	Modularity
1 – 4	1 – (3)(4)/(2*15) = 0.60
4 – 5	1 – (4)(5)/(2*15) = 0.33
5 – 7	1 – (3)(5)/(2*15) = 0.50

Edges with Aij = 0	
1 – 5	0 – (3)(5)/(2*15) = -0.50
1 – 7	0 – (3)(3)/(2*15) = -0.30
4 – 7	0 – (4)(3)/(2*15) = -0.40

Total Modularity Score for Community [1, 4, 5, 7]   0.23

> ### Total Modularity for the two Communities: 0.23 + 0.23 = 0.46
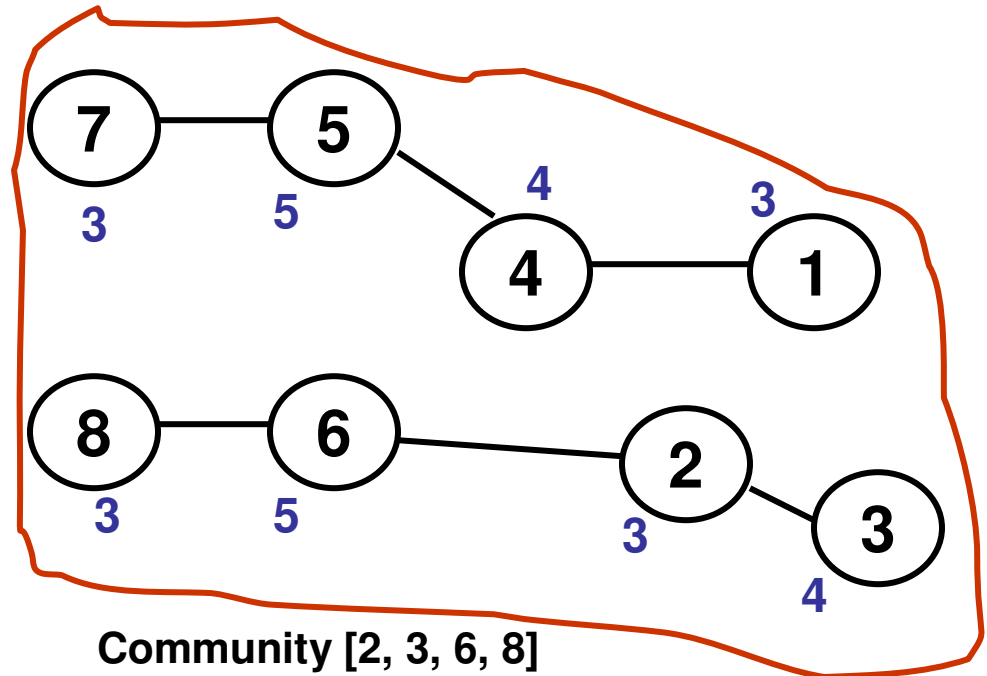
Community [2, 3, 6, 8]

Edges with Aij = 1	Modularity
2 – 3	1 – (3)(4)/(2*15) = 0.60
2 – 6	1 – (3)(5)/(2*15) = 0.50
6 – 8	1 – (3)(5)/(2*15) = 0.50

Edges with Aij = 0	
2 – 8	0 – (3)(3)/(2*15) = -0.30
3 – 6	0 – (4)(5)/(2*15) = -0.67
3 – 8	0 – (4)(3)/(2*15) = -0.40

Total Modularity Score for Community [2, 3, 6, 8]   0. 23

Evaluating Modularity (Example 2)
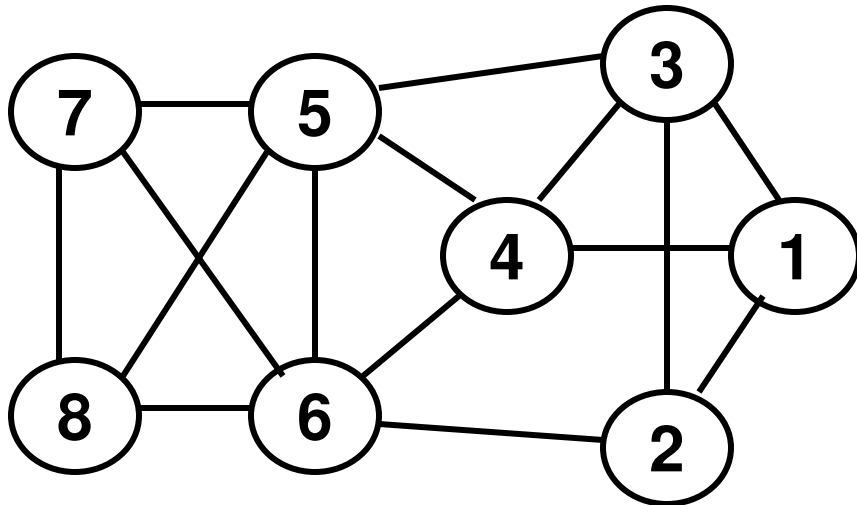
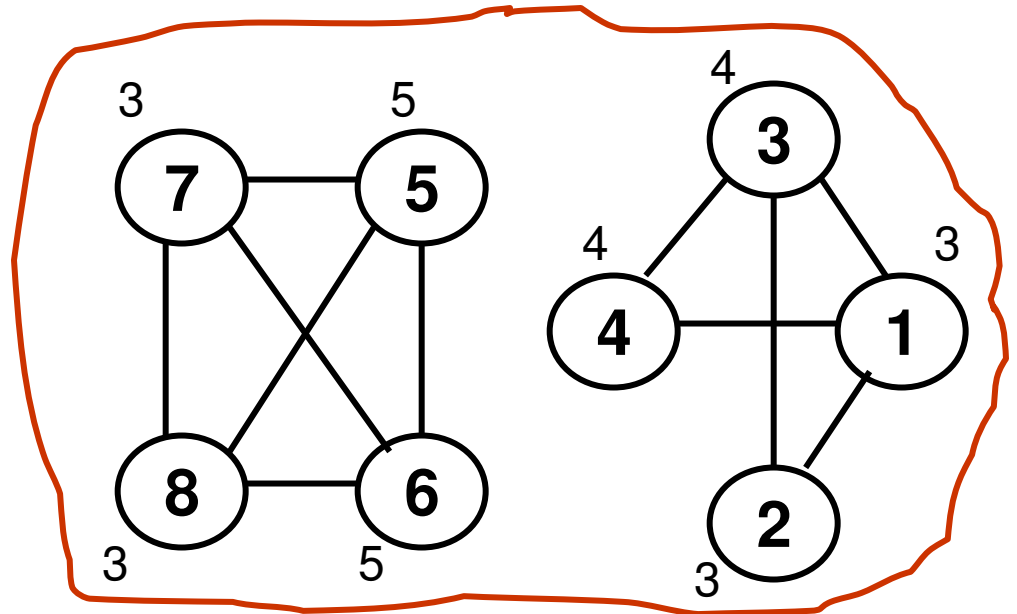**Community [1, 2, 3, 4]**

Edges with Aij = 1	Modularity
1 – 2	1 – (3)(3)/(2*15) = 0.70
1 – 3	1 – (3)(4)/(2*15) = 0.60
1 – 4	1 – (3)(4)/(2*15) = 0.60
2 – 3	1 – (3)(3)/(2*15) = 0.70
3 – 4	1 – (4)(4)/(2*15) = 0.47

Edges with Aij = 0

2 – 4	0 – (3)(4)/(2*15) = -0.40

Total Modularity Score for Community [1, 2, 3, 4]   2.67

Community [5, 6, 7, 8]

Edges with Aij = 1	Modularity
5 – 6	1 – (5)(5)/(2*15) = 0.17
5 – 7	1 – (3)(5)/(2*15) = 0.50
5 – 8	1 – (3)(5)/(2*15) = 0.50
6 – 7	1 – (3)(5)/(2*15) = 0.50
6 – 8	1 – (3)(5)/(2*15) = 0.50
7 – 8	1 – (3)(3)/(2*15) = 0.70

Total Modularity Score for Community [2, 3, 6, 8]   2.87

> **Total Modularity for the two Communities: 2.67 + 2.87 = 5.54**

Using Eigenvectors to Identify Components

- Compute the Eigenvalues and Eigenvectors of the Adjacency matrix A
- The principal Eigenvector is the one that corresponds to the largest Eigenvalue.
- If all the entries in the "principal Eigenvector" are positive, then it implies that all the nodes are in one component.
  - Else, the vertices with the positive entries are in one component and those with the negative entries are in another component. (Note: 0 is considered positive).
- We apply the above interpretation to all the subsequent Eigenvectors (in the decreasing order of the corresponding Eigenvalues) and identify the smaller communities within the larger components.

# Example 1: Eigenvectors to Identify Communities (1)

$$A = \begin{matrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{matrix}$$

1	2
1	3
2	3
3	4
4	5
4	6
5	6
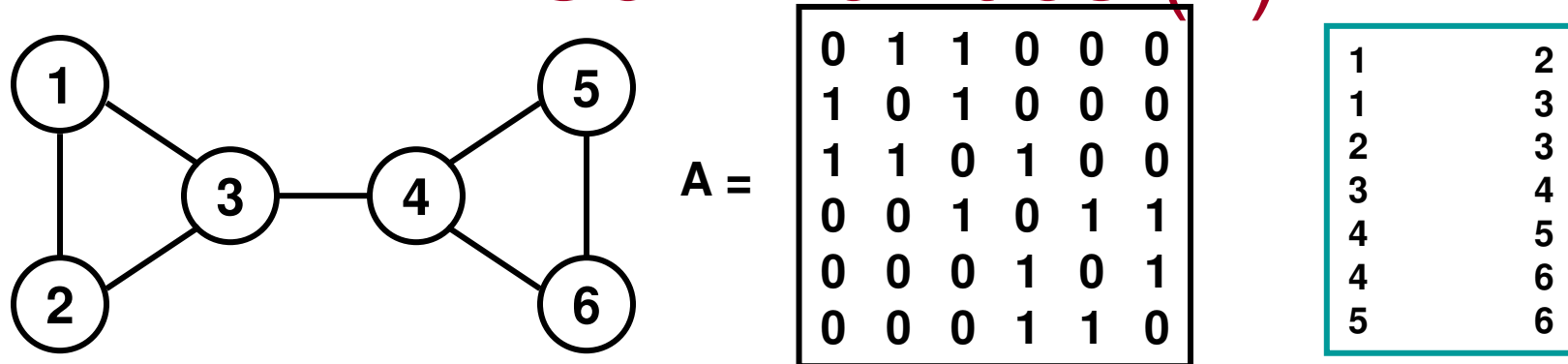
The Eigenvalues in the decreasing order and their corresponding Eigenvectors are:

Eigenvalue	Eigenvector	
2.4142	[0.35; 0.35; 0.5; 0.5; 0.35; 0.35]	All entries are +ve; hence all vertices are in one single component
1.7321	[-0.44; -0.44; -0.33; 0.33; 0.44; 0.44]	Vertices 1, 2, 3 form one community Vertices 4, 5, 6 form another comm.
-0.4142	[0.35; 0.35; -0.5; -0.5; 0.35; 0.35]	Within 1-2-3; 3 is in one comm. Within 4-5-6; 4 is in one comm.
-1	[-0.71; 0.71; 0; 0; 0; 0]	
-1	[0; 0; 0; 0; -0.71; 0.71]	
-1.7321	[0.23; 0.23; -0.63; 0.63; -0.23; -0.23]	

Example 1: Eigenvectors to Identify Communities (2)
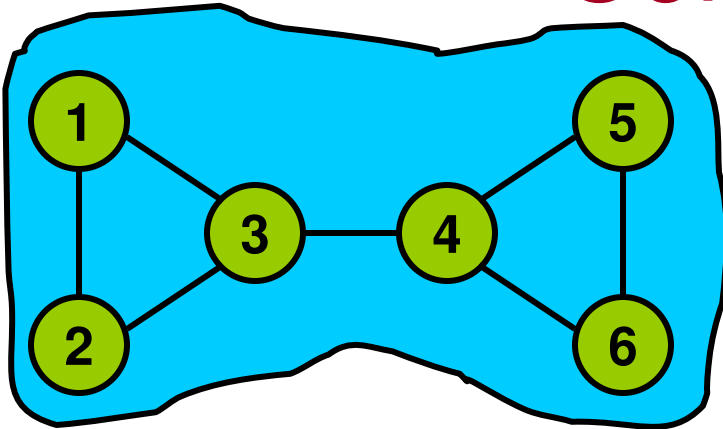
2.4142   [0.35; 0.35; 0.5; 0.5; 0.35; 0.35]
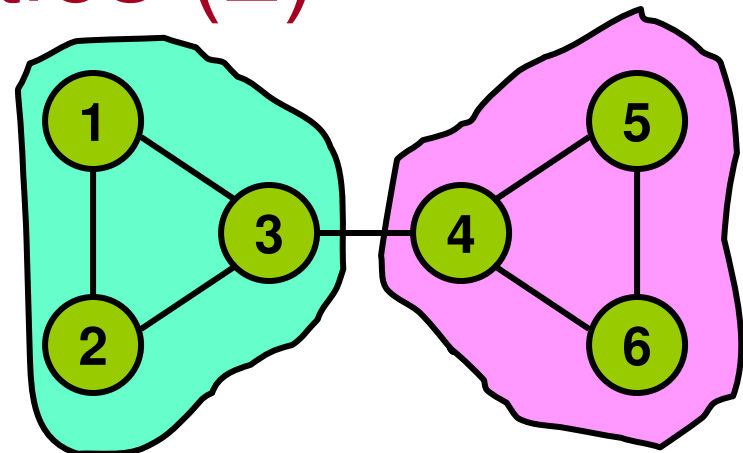
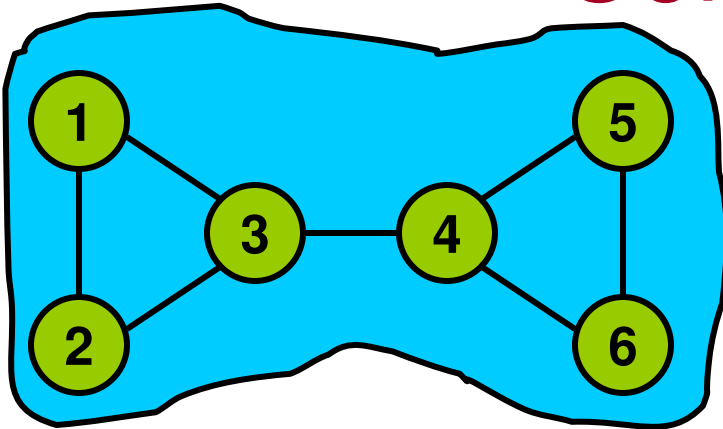1.7321   [-0.44; -0.44; -0.33; 0.33; 0.44; 0.44]

Modularity of [1, 2, 3]

Edge	Modularity
1 – 2	$1 - \{(2*2)/(2*7)\} = 0.71$
1 – 3	$1 - \{2*3)/(2*7)\} = 0.57$
2 – 3	$1 - \{(2*3)/(2*7)\} = 0.57$
Total Modularity = **1.85**	

Modularity of [4, 5, 6]

Edge	Modularity
4 – 5	$1 - \{(2*3)/(2*7)\} = 0.57$
4 – 6	$1 - \{2*3)/(2*7)\} = 0.57$
5 – 6	$1 - \{(2*2)/(2*7)\} = 0.71$
Total Modularity = **1.85**	

Total Modularity of [1, 2, 3] and [4, 5, 6] = <u>3.7</u>

Example 1: Eigenvectors to Identify Communities (3)
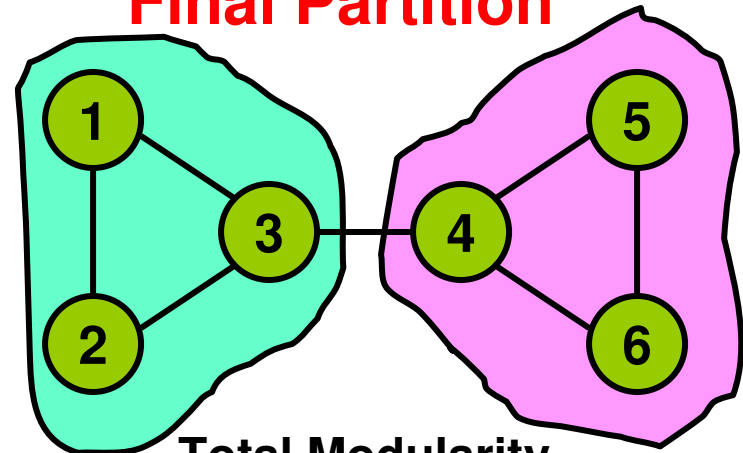

2.4142   [0.35; 0.35; 0.5; 0.5; 0.35; 0.35]
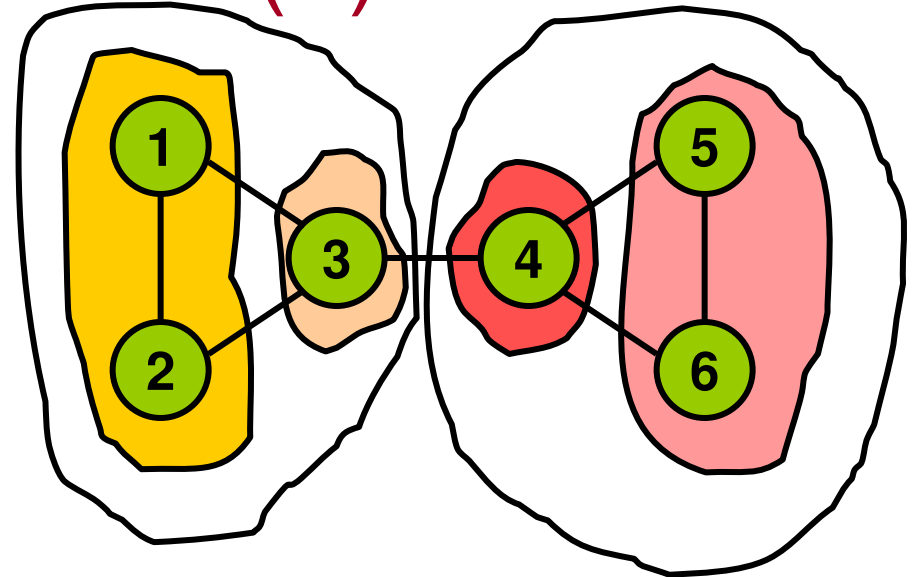
Modularity of [3] and [4] are 0 each
Modularity of [1, 2] and [5, 6] are 0.71 each

Total Modularity of [1, 2] and [3] is 0.71
is less than the modularity of [1, 2, 3]. Hence,
We stay with [1, 2, 3] as a community.

Total Modularity of [5, 6[and [4] is 0.71
is less than the modularity of [4, 5, 6]. Hence,
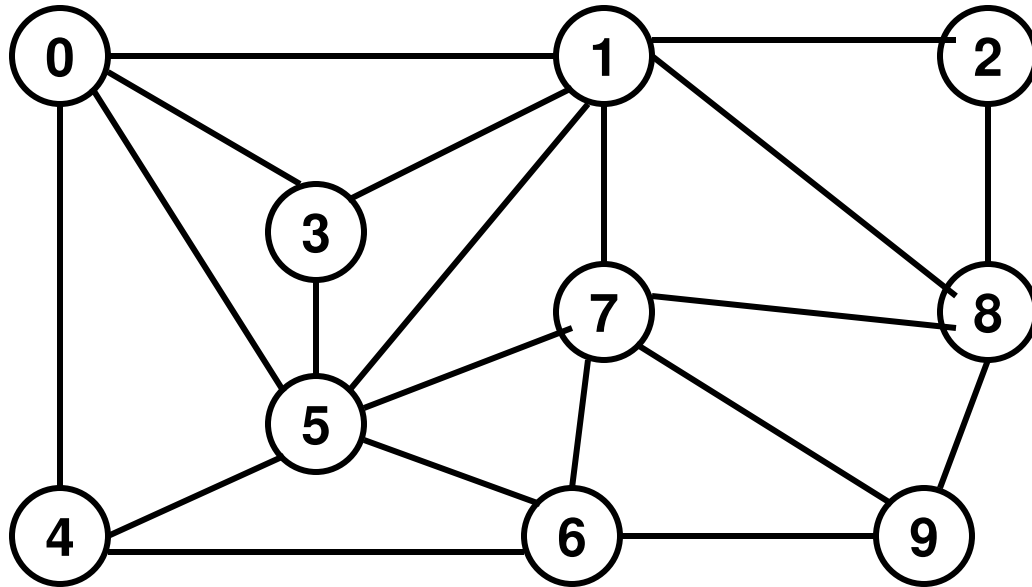We stay with [4, 5, 6] as a community.

Final Partition

Total Modularity
Score = 3.7

Example 2

Eigenvalue # 10 (4.3515)

```
0  0.319710270928999
1  0.426420098753327136
2  0.160703528303939387
3  0.274067807962952
4  0.244256778523456567
5  0.446482529766949б
6  0.296966608945022
7  0.381728429845956
8  0.272885311344487964
9  0.218615358909482
```
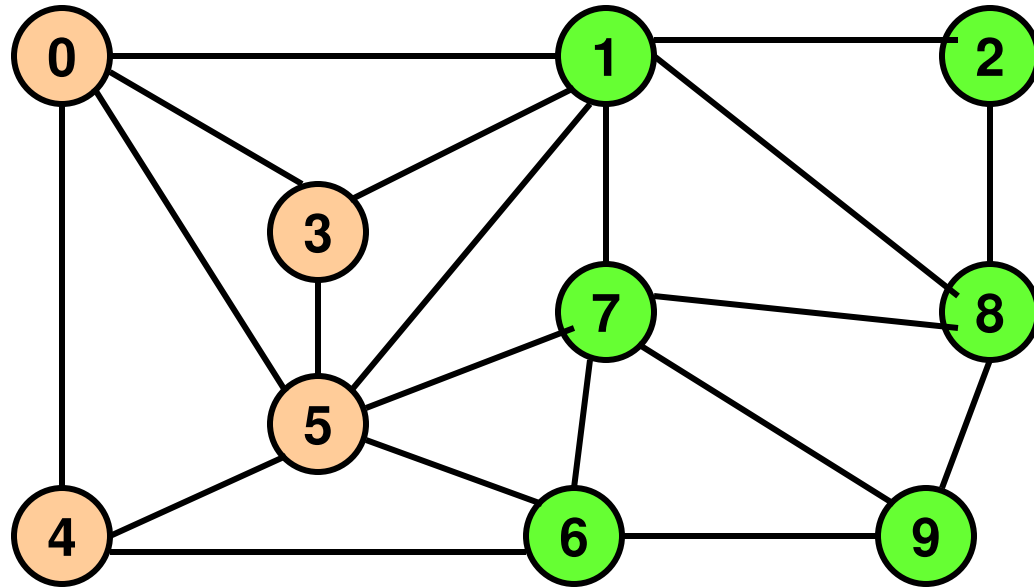
Eigenvalue # 9 (2.1175)

```
0  -0.414785230820025494
1   0.003448307134804475
2   0.221308082070367553
3  -0.324654904415762454
4  -0.28097915591550676
5  -0.276112087029933
6   0.095930654770678
7   0.336379564509900897
8   0.465166279849068
9   0.42384525877557
```

Eigenvalue # 8 (1.6723)

```
0   0.1164837679157984
1   0.430514608467686
2   0.407558199377708554
3   0.242122540021507454
4  -0.335742360646069
5  -0.142098283222588
6  -0.53584669923741234
7  -0.155162707963287164
8   0.25104348443917357
9  -0.26309093820736645
```

Example 2 (1)

```
0 -0.414785230B2002594
1  0.0034483071344804475
2  0.22130B0B207036753
3 -0.32465490044157624
4 -0.28097915591550676
5 -0.27611208702933
6  0.09593065477768678
7  0.33637956450900897
8  0.46516627984900688
9  0.423B4255258775577
```
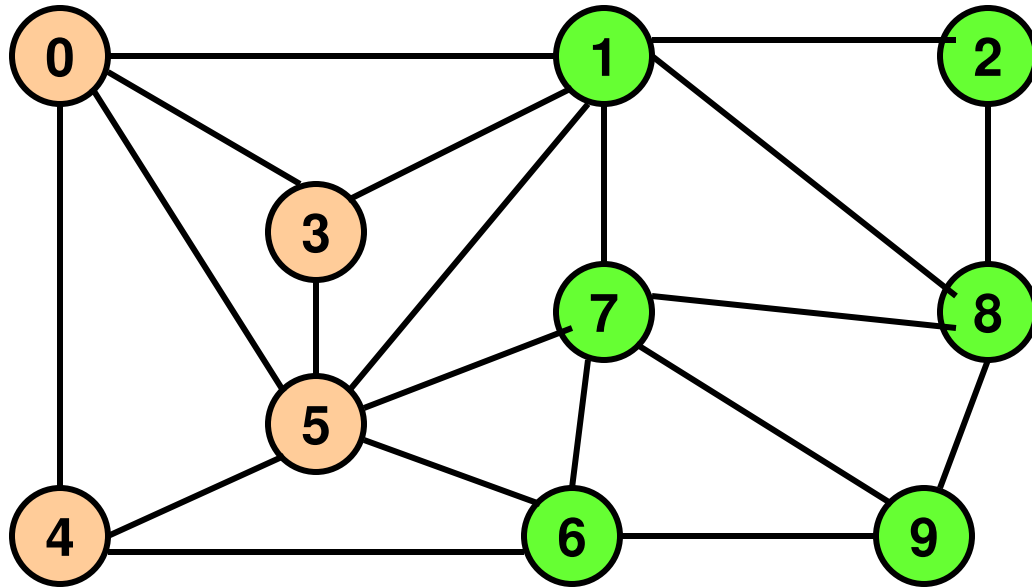
Modularity for Community [0, 3, 4, 5]

Edge	Modularity
0 – 3	1 – {(4*3)/(2*20)} = 0.7
0 – 4	1 – {(4*3)/(2*20)} = 0.7
0 – 5	1 – {(4*6)/(2*20)} = 0.4
3 – 4	0 – {(3*3)/(2*20)} = -0.23
3 – 5	1 – {(3*6)/(2*20)} = 0.55
4 – 5	1 – {(3*6)/(2*20)} = 0.55

Total Modularity Score for
[0, 3, 4, 5] = **2.67**

Modularity for Community [1, 2, 6, 7, 8, 9]

Edge	Modularity
1 – 2	1 – {(6*2)/(2*20)} = 0.7
1 – 6	0 – {(6*4)/(2*20)} = -0.6
1 – 7	1 – {(6*5)/(2*20)} = 0.25
1 – 8	1 – {(6*4)/(2*20)} = 0.4
1 – 9	0 – {(6*3)/(2*20)} = -0.45
2 – 6	0 – {(2*4)/(2*20)} = -0.2
2 – 7	0 – {(2*5)/(2*20)} = -0.25
2 – 8	1 – {(2*4)/(2*20)} = 0.8

Example 2 (2)

Modularity for Community
[1, 2, 6, 7, 8, 9]

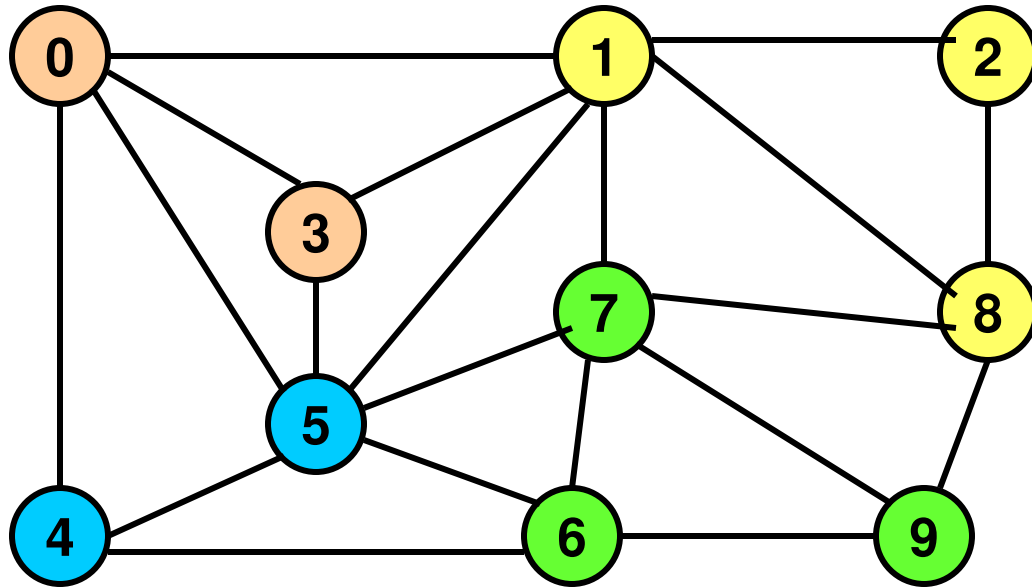| Edge	Modularity
1 – 2	$1 - \{(6*2)/(2*20)\} = 0.7$
1 – 6	$0 - \{(6*4)/(2*20)\} = -0.6$
1 – 7	$1 - \{(6*5)/(2*20)\} = 0.25$
1 – 8	$1 - \{(6*4)/(2*20)\} = 0.4$
1 – 9	$0 - \{(6*3)/(2*20)\} = -0.45$
2 – 6	$0 - \{(2*4)/(2*20)\} = -0.2$
2 – 7	$0 - \{(2*5)/(2*20)\} = -0.25$
2 – 8	$1 - \{(2*4)/(2*20)\} = 0.8$
2 – 9	$0 - \{(2*3)/(2*20)\} = -0.15$
6 – 7	$1 - \{(4*5)/(2*20)\} = 0.5$
6 – 8	$0 - \{(4*4)/(2*20)\} = -0.4$
6 – 9	$1 - \{(4*3)/(2*20)\} = 0.7$
7 – 8	$1 - \{(5*4)/(2*20)\} = 0.5$
7 – 9	$1 - \{(5*3)/(2*20)\} = 0.63$
8 – 9	$1 - \{(4*3)/(2*20)\} = 0.7$

Total Modularity Score for
[1, 2, 6, 7, 8, 9] = **3.13**

Example 2 (3)

Eigenvalue # 8 (1.6723)

0 0.116484376 79157984
1 0.430514460 84677686
2 0.407558199 37708554
3 0.242122540 0215074
4 -0.335742360 6460691
5 -0.142098283 2225889
6 -0.535846699 2374123
7 -0.155162707 96328716
8 0.251043484 43917357
9 -0.263090938 20736645

Modularity of Community [0, 3] = 0.7
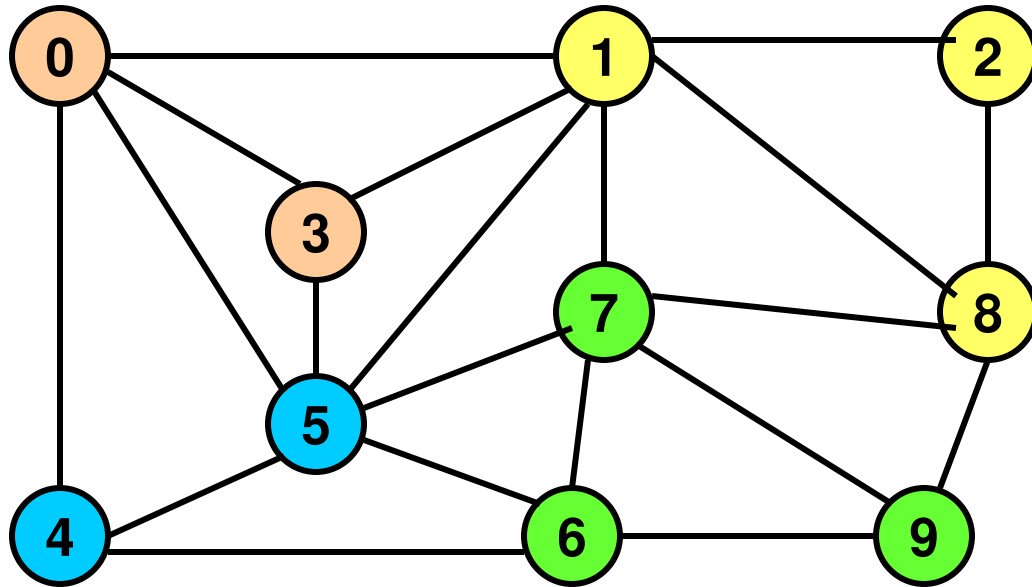**Modularity of Community [4, 5] = 0.55**
Total Modularity of [0, 3] and [4, 5] = 1.25
is less than the Modularity of [0, 3, 4, 5]
= 2.67
Hence, we stay with community [0, 3, 4, 5]
without further partitioning it.

Example 2 (4)

Modularity of Community [1, 2, 8]

Edge	Modularity
1 − 2	1 − {(6*2)/(2*20)} = 0.7
1 − 8	1 − {(6*4)/(2*20)} = 0.4
2 − 8	1 − {(2*4)/(2*20)} = 0.8
Total Modularity of [1, 2, 8] = **1.9**	

Modularity of Community [6, 7, 9]

Edge	Modularity
6 − 7	1 − {(4*5)/(2*20)} = 0.5
6 − 9	1 − {(4*3)/(2*20)} = 0.7
7 − 9	1 − {(5*3)/(2*20)} = 0.63
Total Modularity of [6, 7, 9] = **1.83**	

Modularity of [1, 2, 8] = 1.9
Modularity of [6, 7, 9] = 1.83
Total Modularity of [1, 2, 8] and [6, 7, 9]
= 3.73
is larger than the modularity of
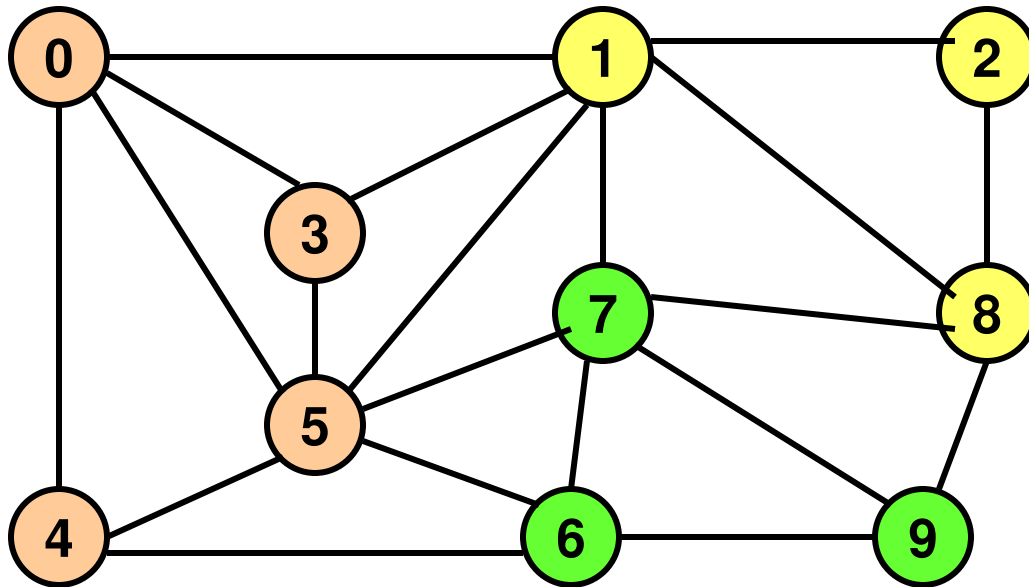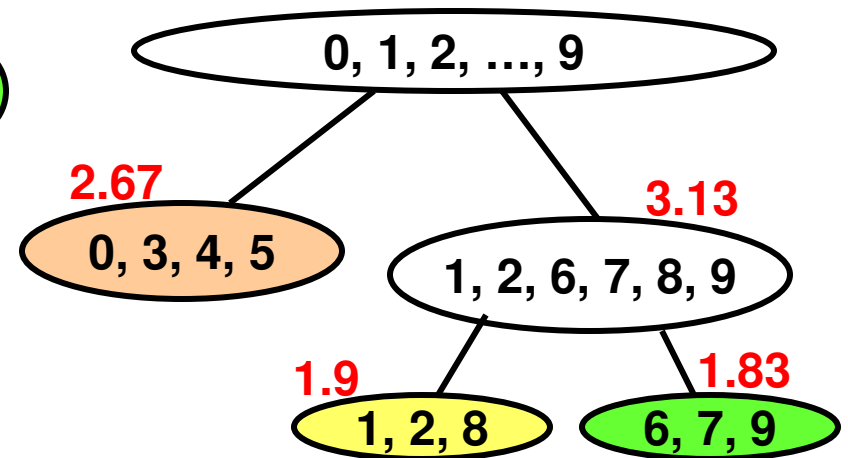[1, 2, 6, 7, 8, 9] = 3.13
Hence, we allow the partitioning of
[1, 2, 6, 7, 8, 9] into [1, 2, 8] and [6, 7, 9]

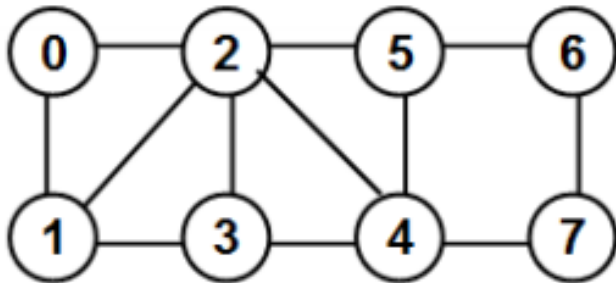# Example 2 (5)

Final Partition

Modularity of [0, 3, 4, 5] = 2.67
Modularity of [1, 2, 8] = 1.9
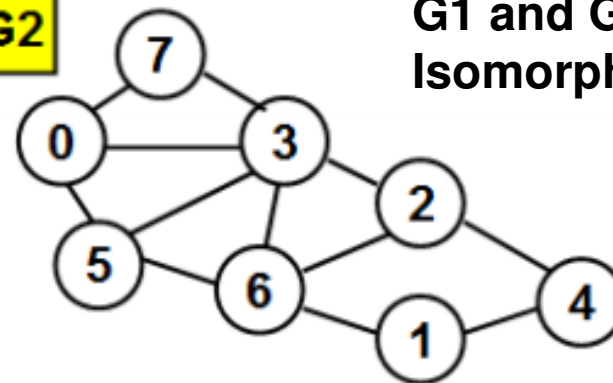Modularity of [6, 7, 9] = 1.83
Total Modularity = 6.4

Graph Isomorphism

- Two graphs are isomorphic if they are structurally similar.
- Two graphs G1 = (V1, E1) and G2 = (V2, E2) are isomorphic if:
  - |V1| = |V2| (i.e., they have the same number of vertices)
  - There exists a one-to-one mapping f of the vertices such that
    - For every vertex v ε V1, f(v) ε V2
    - For every edge (u, v) ε E1, (f(u), f(v)) ε E2.


G1 and G2 are Isomorphic.

Note that determining whether or not two graphs are isomorphic is a NP-hard problem.
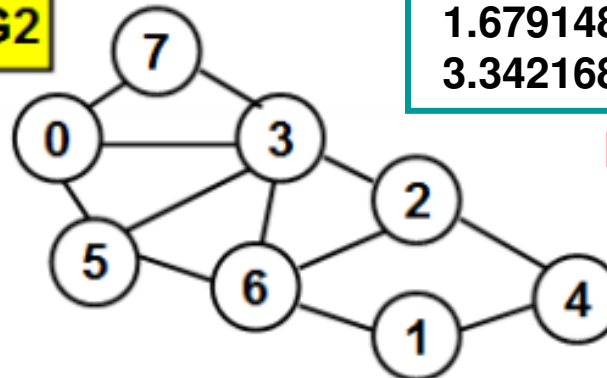
Graph Isomorphism

- Isospectral graphs: Two graphs are said to be isospectral if they have the same eigenvalues.
- If two graphs are isomorphic, they need to be also isospectral, but not vice-versa. Nevertheless, if two graphs are isospectral, they are more likely to be isomorphic.
  - So, spectral analysis can be used as a precursor to test for graph isomorphism.

However, just using the eigenvalues, we cannot determine the one-to-one mapping of the vertices in two isomorphic graphs.
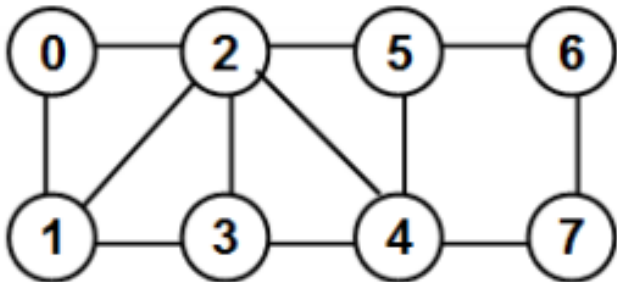
-2.2054526237741263
-1.6597826641247448
-1.4108549659587828
-0.3939833607022455
 0.19153354857068747
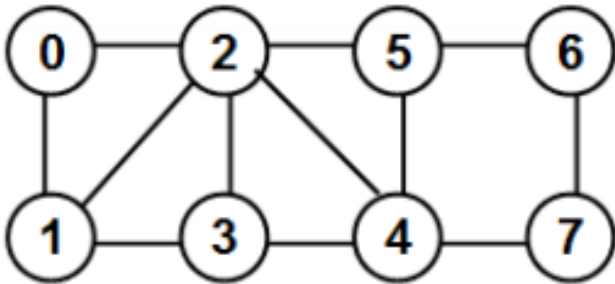 0.4572235096192475
 1.6791484493002504
 3.3421681070697122

Eigenvalues

Principal Eigenvector for Graph Isomorphism

- Two graphs are more likely to be isomorphic if a non-increasing order (or non-decreasing order) of the entries in the principal eigenvector of the two graphs are the same.
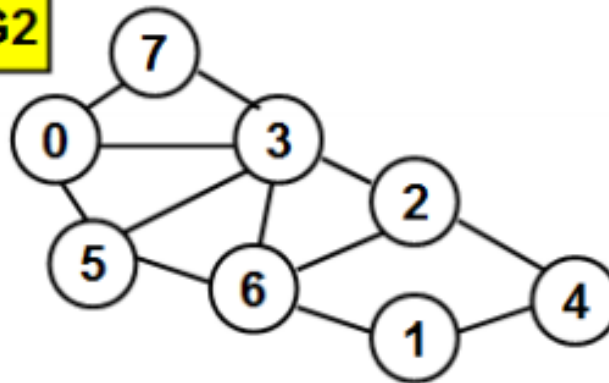

Vertex	Values in the Principal Eigenvector
2	0.5364
4	0.4321
3	0.3974
1	0.3596
5	0.3355
0	0.2681
7	0.1749
6	0.1527

Vertex	Values in the Principal Eigenvector
3	0.5364
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1	0.1749
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Mapping of the Vertices

G1	G2		G1	G2
0	7		5	2
1	0		6	4
2	3		7	1
3	5			
4	6			

Using Degree vs. Principal Eigenvector

- For graphs to be isomorphic, their degree sequence (in non-increasing order or non-decreasing order) should be the same.
- But, if just the non-increasing (or non-decreasing) order of the degree sequence of two graphs are the same, it need not be mean the two graphs are isomorphic. There existed a number of false negatives (i.e., two graphs with identical degree sequence turned out to be non-isomorphic).
- On the other hand, there exists a high probability for two graphs to be isomorphic if they have the same sequence of values (in non-increasing order or non-decreasing order) of the entries in the principal eigenvector.

G1

G2
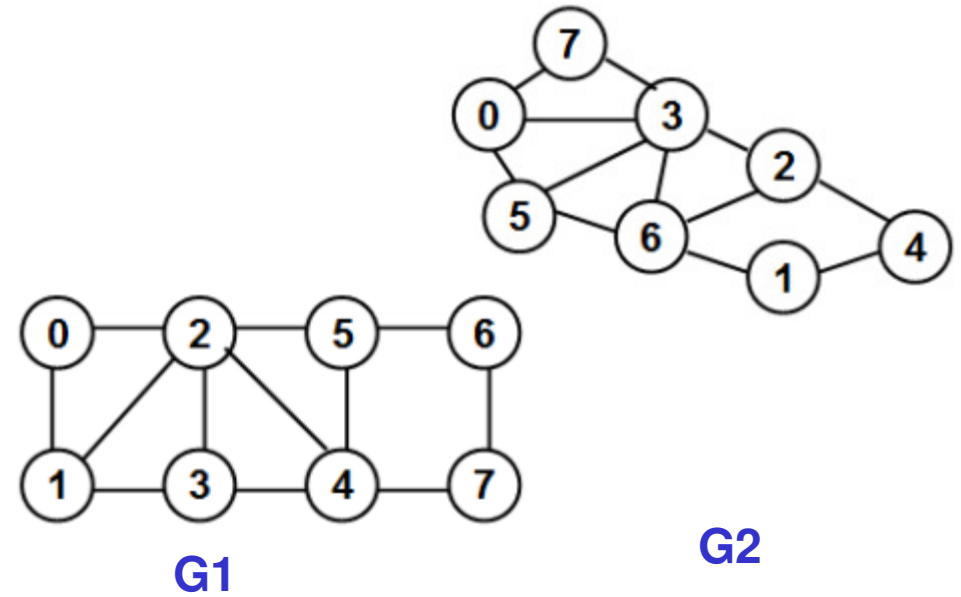
Vertex	Degree	Vertex	Degree
2	5	3	5
4	4	6	4
3	3	5	3
1	3	0	3
5	3	2	3
0	2	7	2
7	2	1	2
6	2	4	2

Degree Sequence: False Negatives
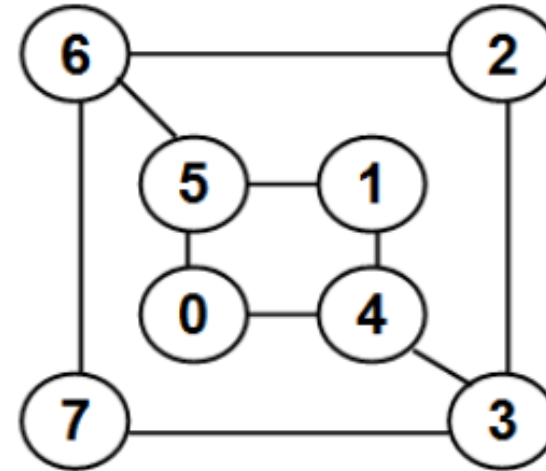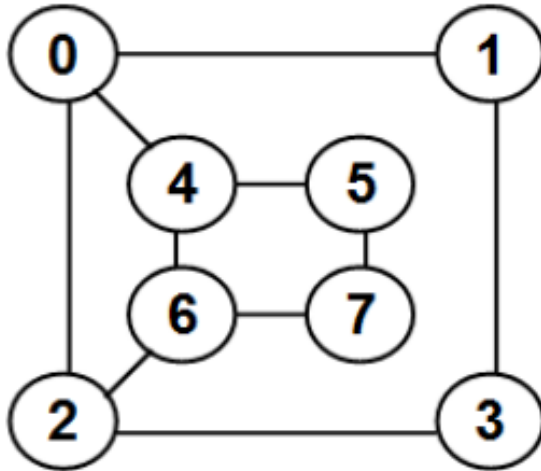
Degree-based Ordering		Principal Eigenvector based Ordering	
Vertex	Degree	Vertex	PEV
0	3	0	0.4253
2	3	2	0.4253
4	3	4	0.4253
6	3	6	0.4253
1	2	1	0.2629
3	2	3	0.2629
5	2	5	0.2629
7	2	7	0.2629

Degree-based Ordering		Principal Eigenvector based Ordering	
Vertex	Degree	Vertex	PEV
3	3	3	0.3941
4	3	4	0.3941
5	3	5	0.3941
6	3	6	0.3941
0	2	0	0.3077
1	2	1	0.3077
2	2	2	0.3077
7	2	7	0.3077

N. Meghanathan, "Exploiting the Discriminating Power of the Eigenvector Centrality Measure to Detect Graph Isomorphism," *International Journal in Foundations of Computer Science and Technology* (IJFCST), vol. 5, no. 6, pp. 1-13, November 2015.
Link: http://wireilla.com/papers/ijfcst/V5N6/5615ijfcst01.pdf