A study on normalized Laplacian, normalized cut and graph partitioning

Kahatapiti Kankanamalage Kissani Ridma, Perera
Graduate School of Mathematics, Kyushu University

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A study on normalized Laplacian, normalized cut and graph partitioning

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By

K.K.Kissani Ridma Perera

Supervisor: Associate Professor Yoshihiro Mizoguchi

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Abstract

In the last decade important relations between the Laplacian eigenvalues and the eigenvectors of graphs and several other graph parameters were discovered. Spectral clustering uses eigenvalues and eigenvectors of matrices associated with graphs to find clusters in the graphs and is widely used to analysis the social networks, web graphs, communication networks etc. In this thesis, we present some of the results and discuss their consequences in spectral clustering and graph energy. We mainly consider normalized Laplacian matrix to find the bipartitions of graphs. Normalized cut introduced by Shi and Malik in 2000 also play a vital role in graph partitioning problems. There is a close relationship between the second smallest eigenvalue of normalized Laplacian matrix and the normalized cut. We compare these two clustering methods and discuss their performances. Besides that we also consider the Laplacian energy of directed graphs, which is also an application of the Laplacian matrices.

First we review the basic terminologies and key results related to Laplacian matrices, which will be used throughout this thesis.

Next we discuss the properties of minimum normalized cut introduced by Shi and Malik for image segmentations. Several authors considered the applications of normalized cut for graph partitioning and less attention is paid for theoretical explanation of this measure compare with isoperimetric and Cheeger constant. Here we use the notation $Mcut(G)$ to represent the minimum normalized cut and derive formula for $Mcut(G)$ of some basic classes of graphs such as paths, cycles, complete graphs, double trees and cycle cross paths and some complex graphs such as lollipop type graphs $LP_{n,m}$ and $LP'_{n,2}$, roach type graphs $R_{n,k}$, weighted paths $P_{n,k}$ and double tree cross paths.

Next we discuss three matrices associated with graphs called difference Laplacian matrix, normalized Laplacian matrix and signless Laplacian matrix and review some known results. Specially we discuss the boundary values of the second smallest eigenvalue of the difference and normalized Laplacian matrices using isoperimetric number and Cheeger constant. Then we derive eigenvalues and eigenvectors of difference, normalized and signless Laplacian matrices of paths and cycles using circulant matrices and give an alternative proof for the eigenvalues of an adjacency matrix of paths and cycles using Chebyshev polynomials. Even most of these results are well known results, we try to summarize them, providing uniform proofs in a simple way.

Next we address the problem of finding graphs which perform poorly on spectral methods. In 1973, Fiedler discussed the possibility of graph partitioning using the sign patterns of second eigenvector of difference Laplacian matrix. Fiedler's investigation was extended by Davies et al. in 2001 using nodal domain theorem. We use the term $Lcut(G)$ to represent the minimum normalized cut of partitions produced by the second eigenvector of normalized Laplacian matrix. Final goal of studying $Mcut(G)$ and $Lcut(G)$ is to investigate the cases, where spectral method perform poorly. More precisely, we give counter examples of graphs and conditions, where $Mcut(G)$ and $Lcut(G)$ produce different clusters on graphs. Especially, we investigate the graphs $R_{n,k}, LP_{n,m}, LP'_{n,2}$ and find conditions, where these two measures make different clusters. We also noticed that the second eigenvector of double tree is an odd vector and therefore we always have $Mcut(DT_n) = Lcut(DT_n)$. This is an exception for the counter examples we discussed under this chapter.

Next we address the problem of finding directed graphs with minimum Laplacian energy. First, we define Laplacian energy of a directed graph as the sum of squares of eigenvalues of a Laplacian matrix defined by using outdegrees of vertices. Then we derive a formula for Laplacian energy of a simple directed graph and show that Laplacian energy of directed graphs can be represented as a sum of squares of outdegrees. Then we consider the class $P(\alpha)$ which consists of non isomorphic graphs with energy less than some positive value α and find 47 non isomorphic directed graphs for class $P(10)$.

Since we can represent the Laplacian energy as a sum of squares of outdegrees of vertices, it motivates us to consider the problem of minimizing sum of squares of degrees in order to find the graph with minimum Laplacian energy. Especially, we studied MMO algorithm introduced by Asahiro 2006, to minimize the maximum outdegree of a directed graph and discuss how far it is applicable to solve our problem and give counter examples, where it is failed. Since the Laplacian energy formula, which we derived is a strict convex function, our problem can be solved by finding optimal semi matching in the bipartite graph.

Finally, we demonstrate the experimental results about spectral clustering on directed graphs. Most real world networks such as network communications, web graphs, social networks etc. are directed and it is worth to analyze the clustering problem in directed graphs. Since a graph constructed by hyper links in web-pages is a directed graph, its adjacency matrix A is asymmetric and does not always have real eigenvalues. Therefore we analyzed the appropriateness of the spectral clustering algorithms on directed graphs. We extend the undirected spectral clustering algorithms to directed graphs using the directed Laplacian matrix introduced by Fan Chung in 2005 and k-means algorithms. Then we compare clustering algorithms based on random walk models and symmetrized transformations. Further we propose an algorithm based on merging techniques. First we apply the directed clustering algorithm and find initial k' number of clusters and then we merge clusters by minimizing normalized cut introduced by Zhou et al. in 2005 for directed graphs until we receive required number of clusters.

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Contents

1 Introduction

1.1 Introduction

Clustering is a common technique in multivariate data analysis, data mining, machine learning etc. The goal of clustering or partitioning problem is to find groups such that entities within the same group are similar and different groups are dissimilar. In the graph partitioning problem much attention is given to seek the precise criteria to obtain a good partition. Clustering methods, which use eigenvalues and eigenvectors of matrices associated with graphs are called spectral clustering and widely used for graph partitioning problems. Specially, eigenvalues and eigenvectors of Laplacian matrices play a vital role in graph partitioning problems. In 1973, Fiedler named the second smallest eigenvalue λ_2 of difference Laplacian matrix as the algebraic connectivity of a graph [16]. In 1975, Fiedler showed that we can decompose a connected graph G into two connected components using only the sign structure of an eigenvector related to the second smallest eigenvalue [17]. Fiedler's investigation was extended by Davies in 2001 using discrete nodal domain theorem [14]. Laplacian matrix, normalized Laplacian matrix and adjacency matrix with negative non diagonal entries can be used with the nodal domain theorem. Nodal domain theorem is useful to identify the number of connected sign graphs of a given graph based on their eigenvectors and eigenvalues. In 1984, Buser investigated the graph invariant quantity $i(G) = \min\limits_{U} \dfrac{cut(U, V \setminus U)}{|U|}$, which considered the relation between the size of the cut and the size of the separated subset U [8]. He called it the isoperimetric number $i(G)$ and the optimal bisection was given by the minimum $i(G)$. Later in 1991, Mohar surveyed the spectrum of difference Laplacian matrix of graphs with special emphasis on the second smallest difference Laplacian eigenvalues $\lambda_2(G)$ and its relation to numerous graph invariants, including connectivity, expanding properties, isoperimetric number, maximum cut, independent number, genus, diameter, mean distance, and bandwidth-type parameters of a graph [35]. Clustering techniques discussed by Wu and Leahy was based on the network flow theory [47]. Minimum cuts in an undirected adjacency graphs are used for partitioning data on large graphs. However this method can be extended to find the partitions in directed network graphs and it is beyond this papers work.

In 1995, Guattery and Miller considered two spectral separation algorithms that partition the vertices based on the values of their corresponding entries in second eigenvector and provide some counter examples for which each of these algorithms produces poor separators [18, 19]. They used eigenvector based on the second smallest eigenvalue of the difference Laplacian matrix as well as a specified number of eigenvector corresponding to the smallest eigenvalues. Finally they used generalized version of spectral methods that allow to use more than a constant number of eigenvector and showed that there are some graphs for which any of the above spectral algorithms perform poorly. We follow their method especially about graph automorphism and even-odd eigenvector theorem for concrete classes of graphs such as roach graphs, double-trees and double tree cross paths. We also describe these properties using formal notations of graphs.

In 1997, Fan Chung discussed most important theories and properties regarding the eigenvalues of normalized Laplacian matrices of graphs and its applications to graph separator problems[10]. She considered partitioning problem using Cheeger constant and derived fundamental relations between eigenvalues and the Cheeger constant. In 2000, Shi and Malik proposed a measure of disassociation called normalized cut for image segmentations [42]. This measure computed the cut cost as a fraction of total edge connections. The normalized cut is used to minimize the disassociation between groups and maximize the association within groups. However minimization of normalized cut criteria is NP hard. Therefore approximate discrete solutions were given. Solution to the minimization problem of normalized cut was given by the second smallest eigenvector of the generalized eigensystem, $(D - W)y = \lambda Dy$, where D is the diagonal matrix with vertex degrees and W is the weighted adjacency matrix. They used minimum normalized cut value as a splitting point and find bisection using second smallest eigenvector. They also noted that eigenvectors are well separated and this kind of splitting point is very reliable. Normalized cut introduced by Shi and Malik is useful for several areas [42]. This measure become interested not only for image segmentation but also for other authors who are interested in network theories and statistics. In 2001, Andrew et al. analyzed the clustering algorithms introduced by Shi and Malik and provided some conditions under which the algorithms work well using matrix perturbation theory [4]. Normalized cut problems were analyzed by Ying Du et al. and provided an approximation algorithm for the minimum normalized cut problem [15]. The theoretical and empirical insight into the nature of the three partitioning measures called minimum, average and normalized cut in terms of the underlying image statistics has been studied by Soundararajan and Sarkar in 2003 [44]. They showed that the normalized cut can be expressed as a sum of two beta distributed random variables, whose parameters are functions of the partition classes. Recently Saralees Nadarajah [37, 36] studied normalized cut from the statistical point of view and derived expressions for mode of the normalized cut. In this thesis, we review several properties of normalized cut and find concrete formula for minimum normalized cut ($Mcut(G)$) of some classes of graphs even this is a NP-hard problem. We also find counter example graphs, where clustering based on normalized Laplacian and normalized cut perform differently.

Eigenvalues of Laplacian matrices play a vital role in mathematical chemistry. Especially in the area of graph energy. Energy has been studied in mathematical perspective as well as physical perspective for several years ago by several authors ([32, 13, 20, 27, 26, 7, 22]). Research on the energy concept dated back to 1940. Coulson evaluated the total energy of π electrons in an unsaturated hydrocarbon molecule [12]. Later, this energy is represented by the sum of absolute values of eigenvalues of adjacency matrices of molecular structure by Ivan Gutman. At the beginning, attention is paid to adjacency matrices and later eigenvalues of several kinds of matrices have been studied, of which Laplacian matrix attracted the greatest attention. Several criteria related to the energy of graphs such as energy change due to edge addition, maximal energy, equal energy has been considered by [3],[27] and [7]. Since molecular graphs have undirected structure, energy and Laplacian energy concept originally developed for undirected graphs. Recently, few authors considered the energy of directed graphs. In 2009, Adiga et al. considered Laplacian energy of directed graphs using skew Laplacian matrix, in which degree of a vertex is the sum of its outdegree and indegree [2, 1]. They extended undirected Laplacian energy to directed graphs by using energy definitions given by [22] and [28]. Further Song et al. use Laplacian energy to find the semantic structures of the image hierarchies of graph, which is an different approach to arranging communities in directed graphs [43]. Most algorithms are developed to minimize the maximum outdegree or maximize the minimum outdegree of an oriented graph. Here we find oriented graph with minimum sum of squares of outdegrees and our approach is based on the Laplacian energy of directed graphs, which is different from the existing approaches.

Extension of undirected clustering algorithms to directed graphs has been considered by several authors. Most real world networks are directed and it is still an unsolved problem for finding efficient clustering algorithms for the directed graphs. In 1999, Kleinberg introduce the framework called 'authority' and 'hub', which separates web page into 2 categories using ranking algorithms, which converges to spectral methods that uses principal eigenvectors of AA^T and A^TA [25]. Different approach called page rank algorithm is used by the Google search engine introduced by Page et al.

with eigenvectors of A itself [40]. In 2005, Zhou et al. used directed spectral clustering method to separate the university web pages into student pages and non-student pages [50]. They extended the normalized cut introduced by Shi and Malik for image segmentation to directed clustering [42]. They used directed Laplacian to find the 2 clusters by using second eigenvector and then they extend the algorithm up to k clusters by minimizing normalized cut values. Leicht and Newman also introduced a modularity function for directed graphs [29]. They first divide the network into two groups using the second eigenvector of the modularity matrix and then divide those groups further by repeated bisection while maximizing the modularity function. The process stops when they reach a point at which further division does not increase the total modularity of the network. This method always use the second eigenvector of modularity matrix for computation and remaining eigenvectors are useless. We extend undirected spectral clustering algorithms to directed graphs by using directed Laplacian matrices. In our method, we first apply directed clustering algorithms to find the initial number of clusters and then merge clusters by minimizing directed normalized cut.

In this thesis, we review the known results about difference Laplacian, normalized Laplacian and signless Laplacian matrices and discuss their applications in the area of graph partitioning and graph energy. We use the term $Mcut(G)$ to represent minimum normalized cut and $Lcut(G)$ to represent normalized cut of the bipartition created by the second eigenvector of normalized Laplacian matrix. This thesis is organized as follows.

Chapter 1 presents basic terminologies and key results related to difference Laplacian, normalized Laplacian and signless Laplacian matrices. We also define graphs using formal notations, which will be used throughout this thesis.

In Chapter 2, we review the properties of $Mcut(G)$ of graphs and derive formula for $Mcut(G)$ of some basic classes of graphs such as paths, cycles, complete graphs, double trees and cycle cross paths and some complex graphs such as lollipop type graphs $LP_{n,m}$, $LP'_{n,2}$, roach type graphs $R_{n,k}$, weighted paths $P_{n,k}$ and double tree cross paths.

In Chapter 3, we survey the known results about difference Laplacian, normalized Laplacian and signless Laplacian matrices. Then we derive eigenvalues and eigenvectors of paths and cycles using three kinds of Laplacian matrices introduced above by using circulant matrices and also give an alternative proof for eigenvalues of adjacency matrices of paths and cycles using Chebyshev formulas.

In Chapter 4, we provide counter examples of graphs on which spectral techniques perform poorly compare with the normalized cut. Especially, we find the conditions for $Mcut(G)$ and $Lcut(G)$ to have different values on the graph $R_{n,k}, LP_{n,m}$ and $LP'_{n,2}$. We also noticed that the second eigenvector of the double tree is odd and $Mcut(DT_n) = Lcut(DT_n)$.

In Chapter 5, we define Laplacian energy of directed graphs using sum of squares of eigenvalues of Laplacian matrices defined by using outdegrees of vertices. Then we obtain a formula for Laplacian energy of simple directed graphs. Next we address the problem of finding oriented graphs with minimum Laplacian energy. We review the existing algorithms for minimizing maximum outdegree of directed graphs such as MMO algorithm and investigate the appropriateness to our problem. We also study bipartite semi matching problems and by joining these two methods, we find the solutions to our problem.

In Chapter 6, we demonstrate experimental results on undirected spectral clustering and directed clustering methods. We extend undirected clustering methods to directed graphs and compare resulted clusters. We also apply the directed clustering methods with merging techniques by minimizing normalized cut.

1.2 Preliminaries

An undirected graph is an ordered pair $G = (V(G), E(G))$, where $V(G)$ is a finite set, elements of which are called vertices, and $E(G)$ is a finite set of unordered pairs of distinct vertices, called edges. We represent $V(G)$ as $V(G) = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E(G)$ as $E(G) = \{(v_i, v_j)|v_i, v_j \in V(G) \textit{ and } v_i, v_j \textit{ are adjacent}\}$. For simplicity, sometimes we use V instead of $V(G)$ and E instead of $E(G)$. For a given subset $S \subseteq V(G)$, $|S|$ represent the size of the set S. For a subset $A \subseteq V(G)$, we represent the set of vertices not belongs to A as $V \setminus A = \{v_i \mid v_i \notin A\}$. A graph $G = (V(G), E(G))$, which has directed edges or arcs is called a directed graph.

Definition 1.1 (Adjacency matrix of an undirected graph)
The adjacency matrix $A(G) = (a_{ij})$ of an undirected graph G is the $n \times n$ matrix whose entries are given by

$$a_{ij} = \begin{cases} 1 & \textit{if } v_i \textit{ and } v_j \textit{ are adjacent,} \\ 0 & \textit{otherwise.} \end{cases}$$

Definition 1.2 (Adjacency matrix of a directed graph)
The adjacency matrix $A(G) = (a_{ij})$ of a directed graph G is the $n \times n$ matrix whose entries are given by

$$a_{ij} = \begin{cases} 1 & \textit{if there exists an arc from } v_i \textit{ to } v_j, \\ 0 & \textit{otherwise.} \end{cases}$$

Definition 1.3 (Simple directed graph)
A directed graph having no multiple edges or self loops is called a simple directed graph. That is $a_{ij} \in \{0, 1\}$ and $a_{ij} = 1 \Rightarrow a_{ji} = 0$.

Definition 1.4 (Symmetric directed graph)
A graph in which each edge is bidirected is called a symmetric directed graph. That is $a_{ij} = 1 \Rightarrow a_{ji} = 1$.

Definition 1.5 (Degree)
The degree of a vertex v_i is defined as $d_i = \sum_{j=1}^{n} a_{ij}$. Minimum and maximum degree of a graph G is denoted by $\delta(G)$ and $\triangle(G)$.

Definition 1.6 (Degree Matrix)
The diagonal matrix of G is denoted by $D(G) = diag(d_1, d_2, \ldots, d_n)$, where d_i is the degree of a vertex v_i.

Note. For simplicity, sometimes we use D instead of $D(G)$.

Definition 1.7 (Volume)
The volume of a graph $G = (V(G), E(G))$ is denoted by $vol(G) = \sum_{i=1}^{|V(G)|} d_i$, is the sum of the degrees of vertices in $V(G)$. Volume of a subset $A \subset V(G)$ is denoted by $vol(A) = \sum_{i \in A} d_i$.

Definition 1.8 (Edge Connectivity)
The edge connectivity of a graph G is denoted by $\kappa'(G)$, is the minimum number of edges needed to remove in order to disconnect the graph. A graph is called k-edge connected if every disconnecting set has at least k edges.

Definition 1.9 (Cartesian product)
The Cartesian product of graphs G and H is denoted by $G\Box H = (V(G\Box H), E(G\Box H))$, where $V(G\Box H) = V(G) \times V(H)$ and $E(G\Box H) = \{(u_1, v_1), (u_2, v_2) \mid u_1 = u_2$ and $(v_1, v_2) \in E(H)$ or $v_1 = v_2$ and $(u_1, u_2) \in E(G)\}$.

Example 1.1 (Cartesian product)
Let C_3 be a cycle graph with $V = \{v_1, v_2, v_3\}$ and P_2 be a path graph with $V = \{x_1, x_2\}$. Then the Cartesian product $C_3\Box P_2$ is shown in the Figure 1.

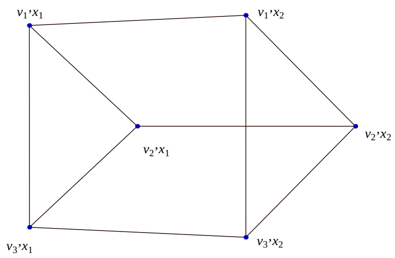


Figure 1: Cartesian product of cycle and path ($C_3\Box P_2$).

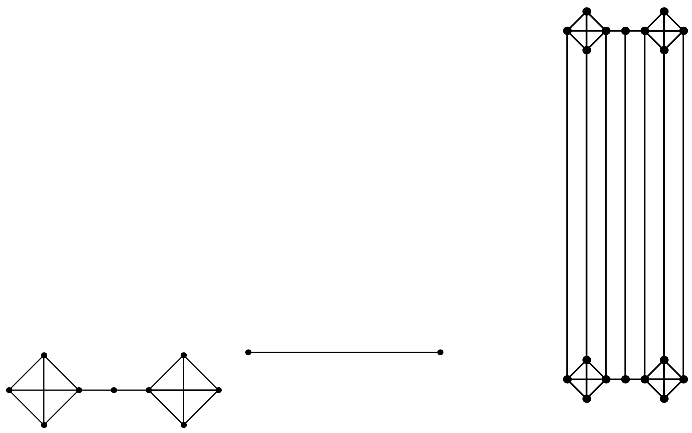
Lemma 1.1 (Xu and Yang 2006 [48])
Let G_1 and G_2 be graphs and $\delta(G_1)$ and $\delta(G_2)$ be minimum degrees of G_1 and G_2. Then $G_1\Box G_2 \cong G_2\Box G_1$ and $\delta(G_1\Box G_2) = \delta(G_1) + \delta(G_2)$.

Theorem 1.1 (Xu and Yang 2006 [48])
If G and H are nontrivial graphs, then $\kappa'(G\Box H) = \min\{\kappa'(G)|V(H)|, \kappa'(H)|V(G)|, \delta(G) + \delta(H)\}$.

■

Example 1.2 (Possibility of $\kappa'(G\Box H) < \delta(G) + \delta(H)$.)
The graph G shown in the Figure 2(a) has $\kappa'(G) = 1, \delta(G) = 2$ and the graph H shown in the Figure 2(b) has $\kappa'(H) = 1, \delta(H) = 1$. Then $\delta(G) + \delta(H) = 3$. The graph $G\Box H$ shown in the Figure 2(c) has $\kappa'(G\Box H) = 2$. For this graph, we have $\delta(G) + \delta(H) > \kappa'(G\Box H)$. ■

Definition 1.10 (Diameter)
Let $G = (V(G), E(G))$ be a graph. The distance between two vertices $v_i, v_j \in V(G)$ of the graph G is denoted by $dist(i, j)$ is the length of a shortest path between vertex v_i and v_j. Maximum distance between any pair of vertices of the graph is called diameter and denoted by $diam(G)$.



(a) G (b) H (c) $G\square H$

Figure 2: Edge connectivity for $G\square H$.

Definition 1.11 (Permutation matrix)
Let $G = (V(G), E(G))$ be a graph. The permutation ϕ defined on $V(G)$ can be represented by a permutation matrix $P = (p_{ij})$, where

$$p_{ij} = \begin{cases} 1 & \text{if } v_i = \phi(v_j), \\ 0 & \text{otherwise.} \end{cases}$$

Definition 1.12 (Automorphism)
Let $G = (V(G), E(G))$ be a graph. Then a bijection $\phi : V(G) \to V(G)$ is an automorphism of G if it preserves the adjacency relation of G. In other words automorphisms of G are the permutations of a vertex set $V(G)$ that maps edges onto edges.

Proposition 1.1 (Biggs [6])
Let $A(G)$ be the adjacency matrix of a graph G, and P be the permutation matrix of permutation ϕ defined on $V(G)$. Then ϕ is an automorphism of G if and only if $PA = AP$.

(Proof) Let $v_h = \phi(v_i)$ and $v_k = \phi(v_j)$. Then we have $(PA)_{hj} = \sum_{l=1}^{n} p_{hl}a_{lj} = a_{ij}$ and $(AP)_{hj} = \sum_{l=1}^{n} a_{hl}p_{lj} = a_{hk}$. Consequently, $AP = PA$ if and only if v_i and v_j are adjacent, whenever v_h and v_k are adjacent. That is if and only if ϕ is an automorphism of $V(G)$. ■

Definition 1.13 (Weighted graph)
A weighted undirected graph $G = (V(G), E(G), w)$, where w is a function from the edge set to the real numbers.

Definition 1.14 (Weighted adjacency matrix)
The weighted adjacency matrix $W = (w_{ij})$ is defined as

$$w_{ij} = \begin{cases} w(i,j) & \text{if } (i,j) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The degree d_i of a vertex v_i of a weighted graph is defined by $d_i = \sum_{j=1}^{n} w_{ij}$. Unweighted graphs are special cases, where all edge weights are 0 or 1.

Definition 1.15 (Graph cut)
A subset of edges which disconnects the graph is called a graph cut. Let $G = (V(G), E(G), w)$ be a weighted graph and $W = (w_{ij})$ the weighted adjacency matrix. Then for $A, B \subset V$ and $A \cap B = \emptyset$, the graph cut is denoted by $cut(A, B) = \sum_{i \in A, j \in B} w_{ij}$.

Definition 1.16 (Isoperimetric number)
The isoperimetric number $i(G)$ of a graph G of order $n \geq 2$ is defined as

$$i(G) = \min\{\frac{cut(S, V \setminus S)}{|S|}, S \subset V(G), 0 < |S| \leq \frac{n}{2}\}.$$

Definition 1.17 (Cheeger constant-edge expansion)
Let $G = (V(G), E(G))$ be a graph. For a non empty subset $S \subset V(G)$, define $h_G(S) = \frac{cut(S, V \setminus S)}{\min(vol(S), vol(V \setminus S))}$. Then the Cheeger constant(edge expansion) h_G is defined as $h_G = \min_S h_G(S)$.

Definition 1.18 (Cheeger constant-vertex expansion)
Let $G = (V(G), E(G))$ be a graph. For a non empty subset $S \subset V(G)$, define $g_G(S) = \frac{vol(\delta S)}{\min(vol(S), vol(V \setminus S))}$, where $\delta S = \{v \notin S : (u, v) \in E(G), u \in S\}$. Then the Cheeger constant(vertex expansion) g_G is defined as $g_G = \min_S g_G(S)$.

Remarks. *Here we use notation δS to represent the vertices belong to the set $V \setminus S$, where each vertex is an endpoint of the edge cut set. This notation is different from the $\delta(G)$, which we use to represent the minimum degree of a graph.*

Definition 1.19 (Weighted difference Laplacian)
The **weighted difference Laplacian** *$L(G) = (l_{ij})$ is defined as*

$$l_{ij} = \begin{cases} d_i - w_{ii} & \text{if } v_i = v_j, \\ -w_{ij} & \text{if } v_i \text{ and } v_j \text{ are adjacent and } v_i \neq v_j, \\ 0 & \text{otherwise.} \end{cases}$$

This can be written as $L(G) = D(G) - W(G)$. For an unweighted graph, $L(G) = D(G) - A(G)$.

Definition 1.20 (Weighted normalized Laplacian)
The **weighted normalized Laplacian** *$\mathcal{L}(G) = (\ell_{ij})$ is defined as*

$$\ell_{ij} = \begin{cases} 1 - \frac{w_{jj}}{d_j} & \textit{if } v_i = v_j, \\ -\frac{w_{ij}}{\sqrt{d_i d_j}} & \textit{if } v_i \textit{ and } v_j \textit{ are adjacent and } v_i \neq v_j, \\ 0 & \textit{otherwise.} \end{cases}$$

Theorem 1.2
Let G be a graph. Then $\mathcal{L}(G) = D^{-1/2}L(G)D^{-1/2}$.

(Proof) Let $T = (t_{ij})_{nn}$, $L(G) = (l_{uv})_{nn}$ and $\mathcal{L}(G) = (\ell_{uv})_{nn}$. Then define

$$t_{ij} = \begin{cases} \frac{1}{\sqrt{d_i}} & v_i = v_j, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$l_{ij} = \begin{cases} d_i & \text{if } v_i = v_j, \\ -1 & (v_i, v_j) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Let $m_{ij} = \sum_{k=1}^{n} t_{ik}.l_{kj}$, where $i = 1, \ldots, n$ and $j = 1, \ldots, n$. If $i \neq k$ then $t_{ik} = 0$ and $m_{ij} = 0$. If $i = k$ then $m_{ij} = t_{ii}.l_{ij}$. Now let $\ell_{ij} = \sum_{k=1}^{n} m_{ik}.t_{kj}$. If $k \neq j$ then $t_{kj} = 0$. If $k = j$, then $\ell_{ij} = m_{ij}.t_{jj}$. Now we can write ℓ_{ij} as $\ell_{ij} = (t_{ii}.l_{ij}).t_{jj} = \frac{1}{\sqrt{d_i}}.l_{ij}\frac{1}{\sqrt{d_j}}$.
Now consider the following cases.

1. If $i = j$ then $\ell_{ii} = \frac{1}{\sqrt{d_i}}.l_{ii}.\frac{1}{\sqrt{d_i}} = 1$,
2. if $(i, j) \in E(G)$ then $\ell_{ij} = \frac{1}{\sqrt{d_i}}.(-1).\frac{1}{\sqrt{d_j}} = \frac{-1}{\sqrt{d_i d_j}}$,
3. Otherwise $l_{ij} = 0$ and $\ell_{ij} = 0$.

By substituting $T = D^{-1/2}$, we get $\mathcal{L}(G) = (\ell_{ij}) = D^{-1/2}LD^{-1/2}$. Further we can deduce $\mathcal{L}(G)$ as $\mathcal{L}(G) = D^{-1/2}LD^{-1/2} = D^{-1/2}(D - W)D^{-1/2} = I - D^{-1/2}WD^{-1/2}$. ■

Definition 1.21 (Signless Laplacian)
The **weighted signless Laplacian** *$SL(G) = (sl_{ij})$ is defined as*

$$sl_{ij} = \begin{cases} d_i + w_{ii} & \textit{if } v_i = v_j, \\ w_{ij} & \textit{if } v_i \textit{ and } v_j \textit{ are adjacent and } v_i \neq v_j, \\ 0 & \textit{otherwise.} \end{cases}$$

We write this as $SL(G) = D + W$.

Matrix M	$M(P_4)$
Adjacency	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
Difference Laplacian	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$
Normalized Laplacian	$\begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 1 \end{pmatrix}$
Signless Laplacian	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$

Table 1: Matrices associated with graphs.

Example 1.3
The Table 1 shows adjacency matrix and three Laplacian matrices discussed in the above for path graph P_4.

Lemma 1.2
Let $G = (V(G), E(G), w)$ be a weighted graph. Then the spectrum of $\mathcal{L}(G)$ and $D^{-1}L(G)$ are equal.

(Proof) $D^{-1}L = D^{-1}(D - W) = I - D^{-1}W = D^{-1/2}DD^{-1/2} - D^{-1/2}D^{-1/2}W = D^{-1/2}(D - W)D^{-1/2}$. Therefore $D^{-1}L(G) = \mathcal{L}(G)$ and has the same spectrum. ∎

Lemma 1.3
Let $\mu_i (i = 1, \ldots, n)$ be the eigenvalues of difference Laplacian matrix $L(G) = D(G) - A(G)$. Then for any regular graph of degree r, normalized Laplacian eigenvalues are $\lambda_i = \dfrac{\mu_i}{r}, (1 \le i \le n)$.

(Proof) $L = (D - A) = rI - A$. *Then* $\mathcal{L}(G) = D^{-1/2}LD^{-1/2} = \dfrac{I}{r^{1/2}}(rI - A)\dfrac{I}{r^{1/2}} = I - \dfrac{A}{r}$. *Then* $r\mathcal{L}(G) = L(G)$. *If μ_i is an eigenvalue of L then it is an eigenvalue of $r\mathcal{L}(G)$. This implies that* $\lambda(\mathcal{L}(G)) = \dfrac{\mu_i}{r}(i = 1, \ldots, n)$. ∎

Proposition 1.2
Let $\mathcal{L}(G)$ be the normalized Laplacian matrix of a graph G and P be the permutation matrix corresponding to the automorphism ϕ defined on $V(G)$. If U is an eigenvector of $\mathcal{L}(G)$ with an eigenvalue λ, then PU is also an eigenvector of $\mathcal{L}(G)$ with the same eigenvalue.

(Proof) From the definition of automorphism, $P^T\mathcal{L}(G)P = \mathcal{L}(G)$. Then $\mathcal{L}(G)U = \lambda U$ implies that $(P^T\mathcal{L}(G)P)U = \lambda U$. Since $PP^T = I$, we get $\mathcal{L}(G)PU = \lambda(PU)$. If U is an eigenvector of $\mathcal{L}(G)$ with an eigenvalue λ then PU is also an eigenvector with the same eigenvalue. ■

Remarks. *This result holds for any matrix associated with a graph under the automorphism defined on a vertex set.*

Definition 1.22 (Odd-even vectors)
Let $G = (V(G), E(G))$ be a graph and $\phi : V \to V$ be an automorphism of order 2. A vector x is called an even vector if $x_i = x_{\phi(i)}$ for all $1 \leq i \leq n$ and a vector y is called an odd vector if $y_i = -y_{\phi(i)}$ for all $1 \leq i \leq n$, where $n = |V(G)|$.

Proposition 1.3
Let G be a graph, ϕ be an automorphism of G with order 2 and P a permutation matrix of ϕ. If an eigenvalue of $\mathcal{L}(G)$ is simple then the corresponding eigenvector is odd or even with respect to ϕ.

(Proof) Let λ be an eigenvalue, U an eigenvector of $\mathcal{L}(G)$. If λ is simple then PU and U are linearly dependent. Then there exists a constant c such that $PU = cU$. Since $P^2 = I$ for an automorphism of order 2, $IU = cPU = c^2U$ and $c = \pm 1$. Then $PU = U$ or $PU = -U$. Hence an eigenvector U is odd or even with respect to ϕ. ■

Definition 1.23
Let $G = (V(G), E(G))$ be a graph, $|V(G)| = n$ and $U = (u_1, u_2, \ldots, u_n)$ an eigenvector of $\mathcal{L}(G)$. We define

$$\begin{aligned} V^+(U) &= \{i \in V \mid u_i > 0\}, \\ V^-(U) &= \{i \in V \mid u_i < 0\} \text{ and} \\ V^0(U) &= \{i \in V \mid u_i = 0\}. \end{aligned}$$

Lemma 1.4
Let $\mathcal{L}(G)$ be the normalized Laplacian of graph G and $U = (u_i), (i = 1, \ldots, n)$ the second eigenvector. If $U \neq \mathbf{0}$ then $V^+(U) \neq \emptyset$ and $V^-(U) \neq \emptyset$.

(Proof) The vector $D^{1/2}\vec{1}$ is an eigenvector corresponding to the zero eigenvalue. Since the second eigenvector U is orthogonal to $D^{\frac{1}{2}}\vec{1}$, $(D^{\frac{1}{2}}\vec{1})^TU = 0$ and $\sum_i \sqrt{d_i}u_i = 0$. Since $d_i > 0, U \neq \mathbf{0}$, there exist at least two values such that $u_i > 0$ and $u_j < 0$ for $i \neq j$. Hence $V^+(U) \neq \emptyset$ and $V^-(U) \neq \emptyset$. ■

Lemma 1.5
Let G be a graph with an automorphism ϕ of order 2. Let $U = (u_1, u_2, \ldots, u_n)$ be an eigenvector and $\phi(U) = (u_{\phi(1)}, u_{\phi(2)}, \ldots, u_{\phi(n)})$. If $U \neq \mathbf{0}$ and $\phi(U) = -U$ then $V^+(U) \neq \emptyset$ and $V^-(U) \neq \emptyset$.

(Proof) Assume $V^+(U) = \emptyset$. If $u_i \leq 0, (i = 1, \ldots, n)$, $\phi(U) = -U$ implies that $u_{\phi(i)} > 0$. This contradicts that $V^+(U) = \emptyset$. Similarly, if we assume that $V^-(U) = \emptyset$ and $u_i \geq 0$ for $(i = 1, \ldots, n)$, then $\phi(U) = -U$ implies that $u_{\phi(i)} < 0$. Then this contradicts that $V^-(U) = \emptyset$. If $u_i = 0, (i = 1, \ldots, n)$, then $U = \mathbf{0}$ and contradicts that $U \neq \mathbf{0}$. ■

Proposition 1.4 (Guattery [18])
Let P_n be a weighted path graph and $\mathcal{L}(P_n)$ be its normalized Laplacian matrix. For any eigenvector $X = (x_1, x_2, \ldots, x_n)$ of $\mathcal{L}(P_n)$,

1. *$x_1 = 0$ implies $X = 0$,*

2. *$x_n = 0$ implies $X = 0$ and*

3. *$x_i = x_{i+1} = 0$ implies that $X = 0$.*

(Proof)

1. *We will give the proof by induction. Let $n = 2$. Then $\mathcal{L}(P_2)X = \lambda X$ can be written as*

$$\begin{pmatrix} \ell_{11} & \ell_{12} \\ \ell_{21} & \ell_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

   Then we have $\ell_{11}x_1 + \ell_{12}x_2 = \lambda x_1 = 0$. If $x_1 = 0$ then $\ell_{12} \neq 0$ implies that $x_2 = 0$, which implies that $X = 0$. For the induction step, assume that the result holds for $\mathcal{L}(P_k)$. Next consider the normalized Laplacian of P_{k+1}. The first entry of the equation of $\mathcal{L}(P_{k+1})X = \lambda X$ is, $\ell_{11}x_1 + \ell_{12}x_2 = \lambda x_1$. Assume that $x_1 = 0$. Then $x_2 = 0$. Let $Y = (y_1, y_2, \ldots, y_k)$ be the vector containing all entries of X except the first entry x_1. Then $x_1 = 0$ implies that $x_2 = y_1 = 0$. Y is an eigenvector of a normalized Laplacian matrix which obtained by deleting first vertex and edge of P_{k+1}. That is this represent the $\mathcal{L}(P_k)$ and satisfy the equation $\mathcal{L}(P_k)Y = \lambda Y$. Since the result holds for all $\mathcal{L}(P_k)$ by induction step, $x_1 = 0$ implies that $Y = 0$ and hence $X = 0$.

2. *Same arguments implies the result for $x_n = 0$.*

3. *Assume that X has two consecutive zeros $x_i = 0$ and $x_{i+1} = 0$. If $i = 1$ or $i+1 = n$ then $X = 0$ by above part 1 and 2 of the proposition. Otherwise, $x_{i+1} = 0$ implies that first i entries of X are zero by the proof of the part 1 of the proposition. Similarly by a symmetric argument, last $n - i$ entries must also be zero, which gives $X = 0$.*

■

Lemma 1.6 (Guattery [18])
For a path graph P_n, $\mathcal{L}(P_n)$ has n simple eigenvalues.

(Proof) Let $U = (u_1, u_2, \ldots, u_n)$ and $\bar{U} = (\bar{u}_1, \bar{u}_2, \ldots, \bar{u}_n)$ be the two eigenvectors of $\mathcal{L}(P_n)$ with the eigenvalue λ. From the Proposition 1.4, we have $u_n \neq 0$ and $\bar{u}_n \neq 0$. Let $\alpha = \dfrac{\bar{u}_n}{u_n}$, where $\alpha \neq 0$. Consider $\mathcal{L}(P_n)(\alpha U - \bar{U}) = \lambda(\alpha U - \bar{U})$. The n-th element of $(\alpha U - \bar{U})$ is $(\bar{u}_n u_n - \bar{u}_n u_n) = 0$. Then $\alpha U = \bar{U}$. Thus U and $\bar{U}$ are linearly dependent, and hence λ is simple. ■

Proposition 1.5
Let $P_n = (V_n, E_n)$ be a path graph with a vertex set $V_n = \{v_1, \ldots, v_n\}$. Let ϕ be an automorphism of order 2 defined on V_n. Then any second eigenvector U_2 of $\mathcal{L}(P_n)$ is an odd-vector.

(Proof) Let λ_2 be the second smallest eigenvalue of $\mathcal{L}(P_n)$. Then $\lambda_2 > 0$ and $U_2 \perp D^{1/2}\vec{1}$. Since λ_2 is simple, any eigenvector U_2 must be even or odd by the Proposition 1.3. Assume U_2 is even. Then $PU_2 = U_2$, where P is the permutation matrix of an automorphism ϕ. From Rayleigh quotient, $\lambda_2 = \min\limits_{U_2 \perp D^{1/2}\vec{1}} \dfrac{U_2^T \mathcal{L}(G) U_2}{U_2^T U_2}$. If n is even, then there exist two center vertices $v_{\frac{n}{2}}$ and $v_{\frac{n}{2}+1}$. If $(U_2)_{\frac{n}{2}} =$

$(U_2)_{\frac{n}{2}+1} = 0$ *then* $U_2 = \mathbf{0}$ *by the Proposition 1.4. Hence* $(U_2)_{\frac{n}{2}} \cdot (U_2)_{\frac{n}{2}+1} \neq 0$. *If* n *is odd, then there exists a single center vertex* $v_{\lceil \frac{n}{2} \rceil}$. *If* n *is odd and* U_2 *is even then the eigenvector entry corresponding to the center vertex may be zero or non-zero. If this is zero, then we can change the signs of all entries with index less than center vertex and form an odd vector such that* $PU_2 = -U_2$. *Thus it contradicts the simplicity of the eigenvalues. Hence we assume that eigenvector entry corresponding to the center vertex is non zero and its value is* c. *Now consider the vector* $X = (-c)\vec{1} + U_2$, *where* $c \neq 0$. *Then the eigenvector entry corresponding to the center vertex of* X *is zero. Now consider*

$$\begin{aligned}
\frac{X^T\mathcal{L}(G)X}{X^TX} &= \frac{((-c)\vec{1}+U_2)^T\mathcal{L}(G)((-c)\vec{1}+U_2)}{((-c)\vec{1}+U_2)^T((-c)\vec{1}+U_2)} \\
&= \frac{c^2.(\vec{1}^T\mathcal{L}(G)\vec{1}) + U_2^T\mathcal{L}(G)U_2 + (\mathcal{L}(G)U_2)^T(-c)\vec{1} + (-c)\vec{1}\mathcal{L}(G)U_2}{c^2n + U_2^TU_2} \\
&= \frac{c^2.(\vec{1}^T\mathcal{L}(G)\vec{1}) + U_2^T\mathcal{L}(G)U_2}{c^2n + U_2^TU_2} \\
&< \frac{U_2^T\mathcal{L}(G)U_2}{U_2^TU_2}.
\end{aligned}$$

We can create an odd vector Y, *by changing the signs of the eigenvector entries above or below the center vertex, such that* $\dfrac{Y^T\mathcal{L}(G)Y^T}{Y^TY} = \dfrac{X^T\mathcal{L}(G)X^T}{X^TX}$ *as follows.* $(Y)_i = (X)_i, i < \dfrac{n}{2}$ *and* $(Y)_i = -(X)_i, i > \dfrac{n}{2}$. *Then* $Y \perp D^{1/2}\vec{1}$ *and has the same eigenvalue* λ_2. *Since* λ_2 *is simple, we have a contradiction. Therefore* U_2 *is an odd eigenvector.* ■

Example 1.4
Let

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

and

$$P = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

If U_M is a second eigenvector of M then by Proposition 1.2, PU_M is also a second eigenvector. By Proposition 1.3, $PU_M = U_M$ or $PU_M = -U_M$. By Proposition 1.5, U_M is an odd vector and $PU_M = -U_M$.

Definition 1.24 (Weighted Path)
Let $P_{n,k} = (P_{ij})$ be the $(n+k) \times (n+k)$ matrix such that

$$P_{ij} = \begin{cases} 0 & (i = j \text{ and } i \leq n) \text{ or } (i \neq j+1 \text{ and } j \neq i+1), \\ 1 & (i = j \text{ and } n+1 \leq i) \text{ or } (i = j+1 \text{ or } j = i+1). \end{cases}$$

Proposition 1.6
Let

$$P_{3,4} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

and

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

If U_M be the second eigenvector of $M = D^{-1/2}(D - P_{3,4})D^{-1/2}$ then $V^+(U_M) \neq \emptyset$ and $V^-(U_M) \neq \emptyset$.

(Proof) Let U_M be the second eigenvector of $\mathcal{L}(M)$. Then by Lemma 1.4, $V^+(U_M) \neq \emptyset$ and $V^-(U_M) \neq \emptyset$. ■

Definition 1.25 (Spectral radius)
Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the (real or complex) eigenvalues of a matrix A. Then the spectral radius $\rho(A)$ is defined as $\rho(A) = \max_i(|\lambda_i|), (i = 1, \ldots, n)$.

Definition 1.26 (Positive-definite)
A symmetric matrix A is called **positive-definite**, *if for all nonzero vectors $x \in \Re^n$ the associated quadratic form given by $A(x) = x^T Ax$ takes only positive values.*

Definition 1.27 (Semidefinite)
If the quadratic form $A(x) = x^T Ax$ takes only non-negative values, then the symmetric matrix A is called **positive-semidefinite**.

Definition 1.28 (Indefinite)
The matrix is indefinite, when it is neither positive-semidefinite nor negative-semidefinite.

Definition 1.29 (Girth)
The girth of a graph is the length of a shortest cycle contained in the graph. If the graph does not contain any cycles (acyclic graph), then the girth is defined to be infinity.

1.3 Formal notations for graphs

Let Σ is an alphabet and Σ^* is a set of strings over Σ including the empty string ϵ. We denote the length of $w \in \Sigma^*$ by $|w|$. Let $\Sigma^{\leq n} = \{w \in \Sigma^* ||w| < n\}$ and $\Sigma_1^{\leq n} = \{w \in \Sigma^* |1 \leq |w| < n\}$. In this paper, we assume $\Sigma = \{0, 1\}$.

Definition 1.30 (Complete binary tree)
A complete binary tree $T_n = (V, E)$ of depth n is defined as follows.

$$\begin{aligned} V &= \Sigma^{\leq n}, \\ E &= E_1 \cup E_2, \\ E_1 &= \{(\epsilon, w) \mid w \in \Sigma_1^{\leq n}, |w| = 1\}, \\ E_2 &= \{(w, wu) \mid w, u \in \Sigma_1^{\leq n}, |wu| < n, |wu| = |w| + 1\}. \end{aligned}$$

Definition 1.31 (Double tree)
A double tree $DT_n = (V, E)$, where n is the depth of the tree, consists of two complete binary trees connected by their root. We define double tree as follows.

$$\begin{aligned} V &= \{x(w) | w \in \Sigma^{\leq n}\} \cup \{y(w) | w \in \Sigma^{\leq n}\}, \\ E_1 &= \{(x(w), x(wu)) \mid w, u \in \Sigma_1^{\leq n}, |wu| < n, |wu| = |w| + 1\}, \\ E_2 &= \{(y(w), y(wu)) \mid w, u \in \Sigma_1^{\leq n}, |wu| < n, |wu| = |w| + 1\}, \\ E_3 &= (x(\epsilon), y(\epsilon)), \\ E_4 &= \{(x(\epsilon), x(w)) \mid w \in \Sigma_1^{\leq n}, |w| = 1\}, \\ E_5 &= \{(y(\epsilon), y(w)) \mid w \in \Sigma_1^{\leq n}, |w| = 1\}, \\ E &= \bigcup_{i=1}^{5} E_i. \end{aligned}$$

Definition 1.32 (Cycle)
A cycle $C_n = (V_n, E_n)$ consists of a vertex set $V_n = \{v_l \mid l \in \mathbb{Z}^+, l \leq n\}$ and an edge set $E_n = \{(v_l, v_{l+1}) \mid 1 \leq l < n\} \cup \{(v_1, v_n)\}$.

Definition 1.33 (Path)
A path $P_n = (V_n, E_n)$ consists of a vertex set $V_n = \{v_l \mid l \in \mathbb{Z}^+, l \leq n\}$ and an edge set $E_n = \{(v_l, v_{l+1}) \mid 1 \leq l < n\}$.

Definition 1.34 (Regular graph)
A graph $G = (V(G), E(G))$ is called r-regular, if degree of each vertex is r.

Definition 1.35 (Complete graph)
A complete graph $K_n = (V_n, E_n)$ consists of a vertex set $V_n = \{v_i \mid 1 \leq i \leq n\}$ and an edge set $E_n = \{(v_i, v_j) \mid i \neq j$ and $1 \leq i \leq n, 1 \leq j \leq n\}$.

Definition 1.36 (Bipartite graph)
A bipartite graph $G = (U, V, E)$ *consists of a vertex set* $U = \{u_i \mid 1 \le i \le m\}$ *and* $V = \{v_i \mid 1 \le i \le n\}$ *and an edge set* $E = \{(u_i, v_j) \mid u_i \in U \text{ and } v_j \in V\}$*, where* $|U| = m$ *and* $|V| = n$*. For simplicity sometimes we use the notation* $K_{m,n}$*, where* m *and* n *are the size of the set* U *and* V*.*

Definition 1.37 (Double tree cross path)
Let DT_n *be a double tree and* P_m *be a path. Then double tree cross path* $(DT_n \Box P_m) = (V, E)$ *is a graph, where*

$$\begin{aligned}
V &= \{(x(w), p(i)) \mid w \in \Sigma^{\le n}, 1 \le i \le m\} \cup \{(y(w), p(i)) \mid w \in \Sigma^{\le n}, 1 \le i \le m\}, \\
E_1 &= \{((x(w), p(i)), (x(wu), p(i))) \mid w \in \Sigma_1^{\le n}, 1 \le i \le m, |wu| = |w| + 1, |wu| < n\}, \\
E_2 &= \{((y(w), p(i)), (y(wu), p(i))) \mid w \in \Sigma_1^{\le n}, 1 \le i \le m, |wu| = |w| + 1, |wu| < n\}, \\
E_3 &= \{((x(w), p(i)), (x(w), p(i+1))) \mid w \in \Sigma^{\le n}, 1 \le i < m\}, \\
E_4 &= \{((y(w), p(i)), (y(w), p(i+1))) \mid w \in \Sigma^{\le n}, 1 \le i < m\}, \\
E_5 &= \{(x(\epsilon), p(i)), (x(w), p(i)) \mid w \in \{0, 1\}, 1 \le i \le m\}, \\
E_6 &= \{(x(\epsilon), p(i)), (y(\epsilon), p(i)) \mid 1 \le i \le m\}, \\
E_7 &= \{(y(\epsilon), p(i)), (y(w), p(i)) \mid w \in \{0, 1\}, 1 \le i \le m\}, \\
E &= E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5 \cup E_6 \cup E_7.
\end{aligned}$$

Definition 1.38 (Graph $R_{n,k}$)
The graph $R_{n,k}(n \ge 1, k \ge 2)$ *is a bounded degree planer graph with a vertex set* $V = V_1 \cup V_2$ *and an edge set* $E = E_1 \cup E_2 \cup E_3$*.*

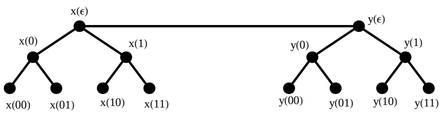
$$\begin{aligned}
V_1 &= \{x_i \mid 1 \le i \le n + k\}, \\
V_2 &= \{y_i \mid 1 \le i \le n + k\}, \\
E_1 &= \{(x_i, x_{i+1}) \mid 1 \le i \le n + k - 1\}, \\
E_2 &= \{(y_i, y_{i+1}) \mid n + k + 1 \le i \le 2(n + k) - 1\}, \\
E_3 &= \{(x_i, y_i) \mid n + 1 \le i \le n + k\}.
\end{aligned}$$

Definition 1.39 (Cycle cross paths $C_m \Box P_n$)
Let C_m *be a cycle with* $V = \{c_i \mid 1 \le i \le m\}$ *and* $E = \{(c_i, c_{i+1}) \mid 1 \le i < m\} \cup \{(c_1, c_m)\}$*. Let* P_n *be a path with* $V = \{p_i \mid 1 \le i \le n\}$ *and* $E = \{(p_i, p_{i+1}) \mid 1 \le i < n\}$*. Graph* $C_m \Box P_n$ *has* n *copies of cycles* C_m*, each corresponding to the one vertex of the path graph. A vertex set* V *and an edge set* $E = E_1 \cup E_2 \cup E_3$ *of* $C_m \Box P_n$ *is defined as follows.*

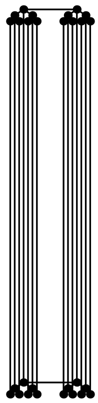
$$\begin{aligned}
V &= \{(c_i, p_j) \mid 1 \le i \le m, 1 \le j \le n\}, \\
E_1 &= \bigcup_{i=1}^{m} \{((c_i, p_j), (c_i, p_{j+1})) \mid 1 \le j \le n - 1\}, \\
E_2 &= \bigcup_{j=1}^{n} \{((c_i, p_j), (c_{i+1}, p_j)) \mid 1 \le i \le m - 1\}, \\
E_3 &= \{((c_i, p_i), (c_m, p_i)) \mid 1 \le i \le n\}, \\
E &= E_1 \cup E_2 \cup E_3.
\end{aligned}$$

Example 1.5

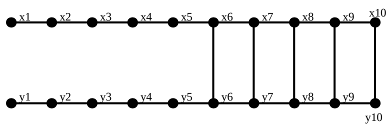
Let $DT_3 = (V, E)$ be a double tree with $V = \{x(\epsilon), x(0), x(1), y(\epsilon), y(0), y(1), x(00), x(01), x(10), x(11), y(00), y(01), y(10), y(11)\}$ and $E = \{(x(\epsilon), y(\epsilon)), (x(\epsilon), x(0)), (x(\epsilon), x(1)), (y(\epsilon), y(0)), (y(\epsilon), y(1)), (x(0), x(00)), (x(0), x(01)), (x(1), x(10)), (x(1), x(11)), (y(0), y(00)), (y(0), y(01)), (y(1), y(10)), (y(1), y(11))$. Then the double tree cross path $DT_3 \square P_2$ is a graph as shown in the Figure 3(b). Graph $R_{5,5}$ is shown in the Figure 3(c) has a vertex set $V = \{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8, y_9, y_{10}\}$ and an edge set $E = \{(x_6, y_6), (x_7, y_7), (x_8, y_8), (x_9, y_9), (x_{10}, y_{10})\}$.



(a) Double Tree DT_3



(b) $DT_3 \square P_2$



(c) $R_{5,5}$

Figure 3: Double tree DT_3, double tree cross path $DT_3 \square P_2$, graph $R_{n,k}(n = 5, k = 5)$.

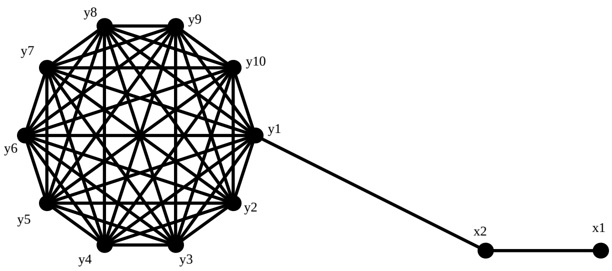
Definition 1.40 (Lollipop graph $LP_{n,m}$)

The lollipop graph $LP_{n,m}, (n \geq 3, m \geq 1)$ is obtained by connecting one vertex of K_n to the end *vertex of P_m as shown in the Figure 4(a). We start vertex numbering from the end vertex of the path. Define $LP_{n,m} = (V, E)$ as follows.*

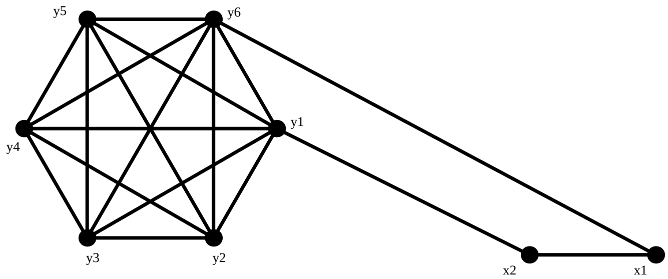
$$\begin{aligned} V &= \{x_1, x_2, \ldots, x_m, y_1, \ldots, y_n\}, \\ E &= \{(x_i, x_{i+1}) \mid 1 \leq i \leq m-1\} \cup \{(y_i, y_j) \mid i \neq j, 1 \leq i \leq n, 1 \leq j \leq n\} \cup \{(x_m, y_1)\}. \end{aligned}$$

Definition 1.41 (Graph $LP'_{n,2}$)
$LP'_{n,2}, (n \geq 3)$ is a graph obtained by connecting both end vertices of P_2 to two adjacent vertices of K_n as shown in the Figure 4(b). The graph $LP'_{n,2} = (V, E)$ is defined as follows.

$$\begin{aligned} V &= \{x_1, x_2, y_1, \ldots, y_n\}, \\ E &= \{(y_i, y_j) \mid i \neq j, 1 \leq i \leq n, 1 \leq j \leq n\} \cup \{(x_1, y_n), (x_2, y_1), (x_1, x_2)\}. \end{aligned}$$



(a) $LP_{10,2}$



(b) $LP'_{5,2}$

Figure 4: Graph $LP_{n,m}(n = 10, m = 2)$ and $LP'_{n,2}(n = 6)$.

2 Minimum normalized cut of some graph classes

We use the term $Mcut(G)$ to represent the minimum normalized cut. In this chapter, we review the basic properties of $Mcut(G)$ and its relation to the connectivity and the second smallest eigenvalue of normalized Laplacian. We also derive $Mcut(G)$ of basic classes of graphs and more complex graphs such as $R_{n,k}$, $P_{n,k}$, $LP_{n,m}$, $LP'_{n,2}$ and $(DT_n \Box P_m)$.

2.1 Properties of $Mcut(G)$

Definition 2.1 (Normalized cut)
Let $G = (V(G), E(G))$ be a graph. Let $A, B \subset V(G)$ and $A \cap B = \emptyset$. Then the normalized cut $Ncut(A, B)$ of G can be written as $Ncut(A,B) = \dfrac{cut(A,B)}{vol(A)} + \dfrac{cut(B,A)}{vol(B)} = cut(A,B)\left(\dfrac{1}{vol(A)} + \dfrac{1}{vol(B)}\right)$.

Definition 2.2 ($Mcut(G)$)
Let $G = (V(G), E(G))$ be a graph and A is a non empty subset of $V(G)$. Then $Mcut(G)$ of a graph G is defined as $Mcut(G) = \min\limits_{A \subset V} Ncut(A, V \setminus A)$.

Example 2.1
The graph $G = (V, E)$ shown in the Figure 5 has a vertex set $V = \{1, 2, 3, 4, 5, 6, 7\}$ and an edge set $E = \{(1, 2), (2, 3), (3, 1), (3, 4), (1, 4), (1, 5), (3, 6), (6, 5), (7, 5), (7, 6)\}$. A volume of G is 20. We compute normalized cut for the subsets taken from G and listed in the Table 2. Considering Case(1),Case(2) and Case(3), we obtain $Mcut(G)$ for the Case(1).

Case	A	$V \setminus A$	$vol(A)$	$vol(V \setminus A)$	$cut(A, V \setminus A)$	$Ncut(A, V \setminus A)$
(1)	$\{1, 2, 3, 4\}$	$\{5, 6, 7\}$	12	8	2	0.417
(2)	$\{1, 2, 3\}$	$\{4, 5, 6, 7\}$	10	10	4	0.8
(3)	$\{1, 3, 4, 5, 6, 7\}$	$\{2\}$	2	18	2	1.1111

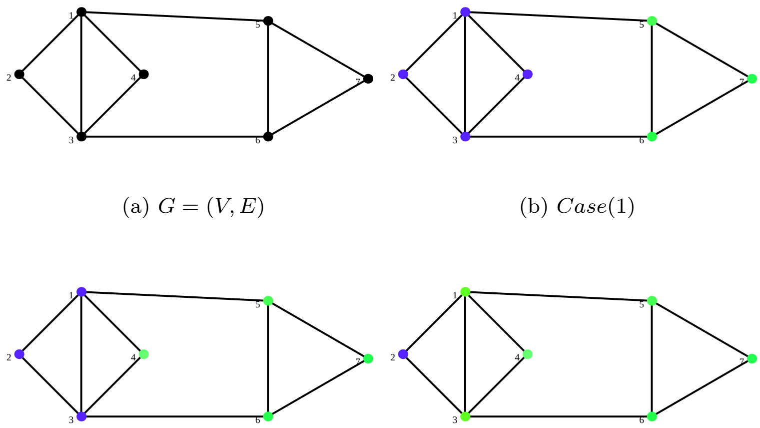
Table 2: Normalized cut.

Lemma 2.1
Let $G = (V(G), E(G))$ be a graph. Then $\left(\dfrac{1}{vol(A)} + \dfrac{1}{vol(V \setminus A)}\right)$ *gives the minimum value, when* $vol(A) = vol(V \setminus A) = \dfrac{vol(G)}{2}$.

■

Proposition 2.1
Let $G = (V(G), E(G))$ be a graph, $A \subseteq V(G)$ and $\triangle(G)$ the maximum degree of G. Then

(i) $cut(A, V \setminus A) \geq \kappa'(G)$.



(a) $G = (V, E)$ (b) $Case(1)$

(c) $Case(2)$ (d) $Case(3)$

Figure 5: Normalized cut- example.

(ii) $Mcut(G) \geq \dfrac{4\kappa'(G)}{\triangle(G)|V(G)|}$.

(iii) *If* $cut(A, V \setminus A) = \kappa'(G)$ *and* $2vol(A) = vol(G)$ *then* $Mcut(G) = \dfrac{4\kappa'(G)}{vol(G)}$.

(Proof)

(i) *Since* $\kappa'(G)$ *is the edge connectivity,* $cut(A, V \setminus A) \geq \kappa'(G)$ *holds for any* $A \subseteq V$.

(ii) *From Lemma 2.1,* $\left(\dfrac{1}{vol(A)} + \dfrac{1}{vol(V \setminus A)}\right)$ *gives the minimum value, when* $vol(A) = vol(V \setminus A)$. *That is* $\left(\dfrac{1}{vol(A)} + \dfrac{1}{vol(V \setminus A)}\right) \geq \dfrac{2}{vol(A)} = \dfrac{4}{vol(G)}$. *Since* $vol(G) = \sum_{i=1}^{|V|} d_i \leq |V(G)|\triangle(G)$, $Ncut(A, V \setminus A) = cut(A, V \setminus A)\left(\dfrac{1}{vol(A)} + \dfrac{1}{vol(V \setminus A)}\right) \geq \dfrac{4\kappa'(G)}{\triangle(G)|V(G)|}$.

(iii) *If* $cut(A, V \setminus A) = \kappa'(G)$ *and* $2vol(A) = vol(G)$ *then it is clear that,* $Mcut(G) = \dfrac{4\kappa'(G)}{vol(G)}$.

■

Proposition 2.2 (Luxburg [46])
Let $G = (V(G), E(G))$ *be a graph and* $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ *be the eigenvalues of* $\mathcal{L}(G)$. *Then* $Mcut(G) \geq \lambda_2(\mathcal{L}(G))$.

(Proof) *Let* $V(G) = \{1, 2, \ldots, n\}$. *Let* $A \subset V(G)$, $g = (g_1, \ldots, g_n) \in \Re^n$ *be an eigenvector and* $g = D^{1/2}f$. *Define* f_i *as*

$$f_i = \begin{cases} a & \text{if } i \in A, \\ -b & \text{if } i \notin A. \end{cases}$$

Then

$$\frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^n f_i^2 d_i} = \frac{2cut(A, V \setminus A)(a+b)^2}{2(a^2 vol(A) + b^2 vol(V \setminus A))}.$$

Choosing $a = vol(V \setminus A)$ *and* $b = vol(A)$ *gives*

$$\begin{aligned} \frac{2cut(A, V \setminus A)(a+b)^2}{2(a^2 vol(A) + b^2 vol(V \setminus A))} &= \frac{cut(A, V \setminus A)(vol(G))^2}{vol(V \setminus A)^2 vol(A) + vol(A)^2 vol(V \setminus A)} \\ &= \frac{cut(A, V \setminus A)(vol(G))^2}{vol(V \setminus A)vol(A)(vol(A) + vol(V \setminus A))} \\ &= \frac{cut(A, V \setminus A)(vol(G))}{vol(V \setminus A)vol(A)} \\ &= cut(A, V \setminus A)\left(\frac{1}{vol(V \setminus A)} + \frac{1}{vol(A)}\right) \\ &= Ncut(A, V \setminus A). \end{aligned}$$

With the choice of f, a, b *we have* $(D\vec{1})^T f = \sum_{i=1}^n d_i f_i = \sum_{i \in A} d_i a - \sum_{i \notin A} d_i b = 0$. *So* $f \perp D\vec{1}$. *Since* $\lambda_2 = \inf_{f \perp D\vec{1}} \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^n f_i^2 d_i}$, *we have* $\lambda_2 \leq \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^n f_i^2 d_i} = \min_A Ncut(A, V \setminus A) = Mcut(G)$. ■

2.2 General properties of $Mcut(G)$

Lemma 2.2
Let $G = (V(G), E(G))$ *be a graph with* $vol(G) \geq 9$. *Suppose there exists a subset* $A \subset V(G)$ *such that* $cut(A, V \setminus A) = 1$ *and* $|vol(A) - vol(G)/2| \leq 3$. *Then there is no subset* $B \subset V(G)$ *such that* $cut(B, V \setminus B) \geq 2$ *and* $Ncut(B, V \setminus B) < Ncut(A, V \setminus A)$. *In particular, the minimum* $Mcut(G)$ *is attained by some* A *with* $cut(A, V \setminus A) = 1$.

(Proof) *Let* $s = vol(G)$. *Then* $2\left(\frac{1}{(s/2)} + \frac{1}{(s/2)}\right) > \left(\frac{1}{(s/2+3)} + \frac{1}{(s/2-3)}\right)$, *if* $s > 6\sqrt{2} = 8.48$. ■

Lemma 2.3
Let $G = (V(G), E(G))$ *be a graph and* $vol(G) \geq 11$. *Suppose there exists a set* $A \subset V(G)$ *such that* $cut(A, V \setminus A) = 2$ *and* $|vol(A) - vol(G)/2| \leq 3$. *Then there is no subset* $B \subset V(G)$ *such that* $cut(B, V \setminus B) \geq 3$ *and* $Ncut(B, V \setminus B) < Ncut(A, V \setminus A)$. *In particular, the minimum* $Mcut(G)$ *is attained by some* A *with* $cut(A, V \setminus A) = 2$.

(Proof) Let $s = vol(G)$. Then $3\left(\frac{1}{(s/2)} + \frac{1}{(s/2)}\right) > 2\left(\frac{1}{(s/2+3)} + \frac{1}{(s/2-3)}\right)$, if $s > 6\sqrt{3} = 10.4$. ■

Lemma 2.4
Let $G = (V(G), E(G))$ be a graph with $vol(G) \geq 6$. Suppose there exists a subset $A \subset V(G)$ such that $cut(A, V \setminus A) = 2$ and $|vol(A) - vol(G)/2| \leq 3$. Suppose there exists no subset $B \subset V(G)$ such that $cut(B, V \setminus B) = 1$ and $|vol(B) - vol(G)/2| \leq \frac{\sqrt{36 + (vol(G))^2}}{2\sqrt{2}}$. Then there is no subset $C \subset V(G)$ such that $cut(C, V \setminus C) \neq 2$ and $Ncut(C, V \setminus C) < Ncut(A, V \setminus A)$. In particular, the minimum $Mcut(G)$ is attained by some A with $cut(A, V \setminus A) = 2$.

(Proof) Let $s = vol(G)$. Consider a subset $B \subset V(G)$ with $cut(B, V \setminus B) = 1$. By the assumption, we have $|vol(B) - vol(G)/2| > k$, where $k = \frac{\sqrt{36 + (vol(G))^2}}{2\sqrt{2}}$. Then $Ncut(B, V \setminus B) = \left(\frac{1}{vol(B)} + \frac{1}{(vol(G) - vol(B))}\right) \geq 2\left(\frac{1}{s/2+k} + \frac{1}{s/2-k}\right) \geq Ncut(A, V \setminus A)$. Consider $C \subset V(G)$ with $cut(C, V \setminus C) \geq 3$. Then $Ncut(C, V \setminus C) \geq \frac{4cut(C, V \setminus C)}{vol(G)} \geq \frac{12}{s} \geq 2\left(\frac{1}{s/2+3} + \frac{1}{s/2-3}\right) = Ncut(A, V \setminus A)$. This shows the required property. ■

Next we derive a formula for the minimum normalized cut $Mcut(G)$ of some elementary classes of graphs.

2.3 $Mcut(G)$ of elementary classes of graphs

Proposition 2.3
Let $G = (V(G), E(G))$ be a graph.

1. *If G is a disconnected graph then $Mcut(G) = 0$.*
2. *If G is a regular graph of degree d and $|V(G)| = n$, then*

$$Mcut(G) \geq \begin{cases} \frac{4}{n} & \text{if } n \text{ is even,} \\ \frac{4n}{(n^2-1)} & \text{if } n \text{ is odd.} \end{cases}$$

3. *For the cycle C_n,*

$$Mcut(C_n) = \begin{cases} \frac{4}{n} & \text{if } n \text{ is even,} \\ \frac{4n}{(n^2-1)} & \text{if } n \text{ is odd.} \end{cases}$$

   This can be written as $Mcut(C_n) = \frac{n}{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$.

4. *For the complete graph K_n,*

$$\begin{aligned} Mcut(K_n) &= \frac{n}{n-1} \\ &= \lambda_2. \end{aligned}$$

5. For the path graph P_n,

$$Mcut(P_n) = \begin{cases} \frac{2}{n-1} & \text{if } n \text{ is even,} \\ \frac{2(n-1)}{n(n-2)} & \text{if } n \text{ is odd.} \end{cases}$$

This can be written as $Mcut(P_n) = \dfrac{2n-2}{4\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 2n + 1}$.

6. For the cycle cross paths $C_m \square P_n$,

$$Mcut(C_m \square P_n) = \begin{cases} \frac{2(2n-1)}{16\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 4n+1} & 2n > m, \\ \frac{nm}{(2n-1)\lfloor \frac{m}{2} \rfloor \lceil \frac{m}{2} \rceil} & 2n \leq m. \end{cases}$$

7. For the double tree DT_n with depth n, $Mcut(DT_n) = \dfrac{2}{2^{n+1}-3}$.

(Proof)

1. Let G_1, G_2 be connected components of G such that $G = G_1 \cup G_2$. Then $cut(V(G_1), V(G_2)) = 0$ and $Ncut(V(G_1), V(G_2)) = 0$. Since $Mcut(G) \leq cut(V(G_1), V(G_2)) \left(\dfrac{1}{vol(V(G_1))} + \dfrac{1}{vol(V(G_2))} \right) = 0$, we have $Mcut(G) = 0$. ■

2. For a regular graph of degree d, $\kappa'(G) = \triangle(G) = \delta(G) = d$. For $A \subset V(G)$, $Ncut(A, V \setminus A) \geq \kappa'(G) \left(\dfrac{1}{d|A|} + \dfrac{1}{(d|V(G) \setminus A|)} \right) = \dfrac{|V(G)|}{|A||V \setminus A|}$. If $cut(A, V \setminus A) = \kappa'(G)$ then we have $Ncut(A, V \setminus A) = \dfrac{|V(G)|}{|A||V \setminus A|}$. $Ncut(A, V \setminus A)$ is minimum, when $|A| = |V \setminus A|$ by the Lemma 2.1.
If $V(G)$ is even then $Mcut(G) \geq \dfrac{4}{|V(G)|} = \dfrac{4}{n}$ by Lemma 2.1.
If $|V(G)|$ is odd then, we can write $|V(G)|$ as $|V(G)| = \dfrac{|V(G)|-1}{2} + \dfrac{|V(G)|+1}{2}$, where $-1 \leq |A| - |V(G) \setminus A| \leq 1$. Then $Ncut(A, V \setminus A) \geq \kappa'(G) \left(\dfrac{2}{d(|V(G)|-1)} + \dfrac{2}{d(|V(G)|+1)} \right) = \dfrac{4|V(G)|}{(|V(G)|+1)(|V(G)|-1)}$. Hence $Mcut(G) \geq \dfrac{4|V(G)|}{(|V(G)|+1)(|V(G)|-1)} = \dfrac{4n}{n^2-1}$. ■

3. Since a cycle graph is a 2-regular graph, $\delta(C_n) = 2 = \kappa'(C_n)$. Let $A \subset V(G)$ and $cut(A, V \setminus A) \geq 2$. Since C_n is a regular graph and $\min cut(A, V \setminus A) = 2$, $Mcut(C_n) = 4/n$ for even n and $Mcut(C_n) = \dfrac{4n}{n^2-1}$ for odd n by above part 2. Further, For even n, $n = \lfloor \dfrac{n}{2} \rfloor = \lceil \dfrac{n}{2} \rceil$ and for odd n, $\dfrac{(n-1)}{2} = \lfloor \dfrac{n}{2} \rfloor$ and $\dfrac{(n+1)}{2} = \lceil \dfrac{n}{2} \rceil$. Combining odd and even cases together we can write $Mcut(C_n)$ as $Mcut(C_n) = \dfrac{n}{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$. ■

4. For a complete graph K_n, $|V| = n$, $\kappa'(K_n) = n-1$ and $vol(K_n) = n(n-1)$. For any subset $A \subset V(K_n)$, we have $vol(A) = |A|(|V|-1)$ and $cut(A, V \setminus A) = |A|(|V|-|A|)$. Then $Ncut(A, V \setminus A) =$

$|A|(|V|-|A|)\left(\frac{1}{|A|(|V|-1)}+\frac{1}{(|V|-|A|)(|V|-1)}\right)=\frac{|V|}{|V|-1}=\frac{n}{n-1}$. *Hence* $Mcut(K_n)=\frac{n}{n-1}$. ■

5. *For a path graph* P_n, $\kappa'(P_n)=1$, $cut(A,V\setminus A)\geq 1$ *and* $vol(P_n)=2n-2$.
Consider the following cases.
Case(i) *Let* $A_1\subset V$ *such that* $A_1=\{v_i\mid 1\leq i\leq\lfloor\frac{n}{2}\rfloor\}$ *and* $V\setminus A_1=\{v_i\mid\lfloor\frac{n}{2}\rfloor+1\leq i\leq n\}$. *A volume of* A_1 *is* $vol(A_1)=2(\lfloor\frac{n}{2}\rfloor)-1$ *and a volume of* $V\setminus A_1$ *is* $vol(V\setminus A_1)=2(\lceil\frac{n}{2}\rceil)-1$. $Ncut(A_1,V\setminus A_1)=\frac{2n-2}{4(\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil)+1-2n}$. *For even* n, $Ncut(A_1,V\setminus A_1)=\frac{2}{n-1}$. *For odd* n, $\lfloor\frac{n}{2}\rfloor=\frac{n-1}{2},\lceil\frac{n}{2}\rceil=\frac{n+1}{2}$. *Then we have* $Ncut(A_1,V\setminus A_1)=\frac{2(n-1)}{n(n-2)}$. *We notice that* $\kappa'(P_n)=1$ *and* $vol(A_1)\leq vol(V\setminus A_1)$.
Case(ii)*Let* $A_{21}=\{v_i\mid 1\leq i\leq l\}$ *and* $A_{22}=\{v_i\mid k\leq i\leq n\}$. *Then consider a set* $A_2=A_{21}\cup A_{22}$ *and* $V\setminus A_2$ *such that* $|A_2|\geq|V\setminus A_2|$. *Then* $cut(A_2,V\setminus A_2)=cut(A_{21},V\setminus(A_{21}\cup A_{22}))+cut(A_{22},V\setminus(A_{21}\cup A_{22}))=2$ *and* $vol(A_2)=2|A_{21}|-1+2|A_{22}|-1=2(|A_2|-1)$. *Therefore* $Ncut(A_2,V\setminus A_2)=\frac{2(2|V|-2)}{(2|A_2|-2)(2|V\setminus A_2|)}$. *Since* $cut(A_2,V\setminus A_2)=2>\kappa'(P_n)$ *and* $vol(A_2)>vol(V\setminus A_2)$, *using Lemma 2.1,* $Ncut(A_2,V\setminus A_2)>Ncut(A_1,V\setminus A_1)$. *Therefore* $Mcut(P_n)=\frac{2n-2}{4(\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil)+1-2n}$. ■

6. *Let* $G=C_m\Box P_n,(n\geq 2,m\geq 3)$ *be a graph which has* n *copies of cycles* C_m, *each corresponding to one vertex of* P_n. $\kappa'(C_m\Box P_n)=\min\{\kappa'(C_m)|V(P_n)|,\kappa'(P_n)|V(C_m)|,\delta(C_m)+\delta(P_n)\}=\delta(C_m)+\delta(P_n)=3$.
Case(i) *Let* $A_1=\{(c_i,p_j)|1\leq j\leq\lfloor\frac{n}{2}\rfloor,1\leq i\leq m\}$ *and* $V\setminus A_1=\{(c_i,p_j)|\lfloor\frac{n}{2}\rfloor+1\leq j\leq n,1\leq i\leq m\}$. *The volume of* A_1 *is* $vol(A_1)=\lfloor\frac{n}{2}\rfloor(vol(C_m)+2m)-m$, $vol(V\setminus A_1)=\lceil\frac{n}{2}\rceil(vol(C_m)+2m)-m$ *and* $cut(A_1,V\setminus A_1)=m$. *Then* $Ncut(A_1,V\setminus A_1)=\frac{m(4mn-2m)}{(\lfloor\frac{n}{2}\rfloor 4m-m)(\lceil\frac{n}{2}\rceil 4m-m)}=\frac{2(2n-1)}{16\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil-4n+1}$. *When* n *is even,* $Ncut(A_1,V\setminus A_1)=\frac{2}{2n-1}$. *When* n *is odd,* $Ncut(A_1,V\setminus A_1)=\frac{2(2n-1)}{(2n-3)(2n+1)}$.
Case(ii) *Let* $A_2=\{(c_i,p_j)\mid 1\leq i\leq\lfloor\frac{m}{2}\rfloor,1\leq j\leq n\}$ *and* $V\setminus A_2=\{(c_i,p_j)\mid\lfloor\frac{m}{2}\rfloor+1\leq i\leq m,1\leq j\leq n\}$. *The volume of* A_2 *is* $vol(A_2)=n\cdot vol(C_{\lfloor\frac{m}{2}\rfloor})+2\lfloor\frac{m}{2}\rfloor(n-1)=2(2n-1)\lfloor\frac{m}{2}\rfloor$ *and* $vol(V\setminus A_2)=2(2n-1)\lceil\frac{m}{2}\rceil$. *The graph cut horizontally through the cycles and we have* $cut(A_2,V\setminus A_2)=2n$. *Hence* $Ncut(A_2,V\setminus A_2)=\frac{nm}{(2n-1)\lfloor\frac{m}{2}\rfloor\lceil\frac{m}{2}\rceil}$. *When* m *is odd,* $\frac{4nm}{(2n-1)(m^2-1)}$ *and when* m *is even,* $\frac{4n}{(2n-1)m}$.
Now compare the Case(i) with Case(ii).

- *If n is even and m is even then,* $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) = \dfrac{2}{2n-1} - \dfrac{4n}{(2n-1)m} = \dfrac{2(m-2n)}{(2n-1)m}$. *If $m \geq 2n$ then $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) \geq 0$.*

- *If n is even and m is odd then,* $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) = \dfrac{2}{2n-1} - \dfrac{4nm}{(2n-1)(m^2-1)} = \dfrac{2(m^2-1)-4nm}{(2n-1)(m^2-1)}$. *If $m > 2n$ then $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) > 0$. If $m = 2n$ then m should be even for any $n \in \mathbf{Z}$ and the equality does not holds.*

- *If n is odd and m is odd then,* $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) = \dfrac{2(2n-1)}{(2n-3)(2n+1)} - \dfrac{4nm}{(2n-1)(m^2-1)} = \dfrac{2(2n-1)^2(m^2-1) - 4nm(2n-3)(2n+1)}{(2n-3)(2n+1)(2n-1)(m^2-1)}$. *Then the numerator* $2(2n-1)^2(m^2-1) - 4nm(2n-3)(2n+1) > 0$, *if $m > 2n$.*

- *If n is odd and m is even then,* $Ncut(A_1, V \setminus A_1) - Ncut(A_2, V \setminus A_2) = \dfrac{2(2n-1)}{(2n-3)(2n+1)} - \dfrac{4n}{(2n-1)m} = \dfrac{2m(2n-1)^2 - 4n(2n-3)(2n+1)}{(2n-3)(2n+1)(2n-1)m}$. *Then the numerator* $2m(2n-1)^2 - 4n(2n-3)(2n+1) \geq 0$, *if $m \geq 2n$.*

If $m \geq 2n$ then $Case(ii) < Case(i)$, and partition the graph by cutting through cycles. If $m < 2n$ then $Case(i) < Case(ii)$, and partition the graph by cutting through paths. ■

7. *The size of a tree is $|T_n| = 1 + 2 + \cdots + 2^n = 2^n - 1$ and the size of a double tree is $|DT_n| = 2|T_n| = 2^{n+1} - 2$. The volume of a tree is $vol(T_n) = 2vol(T_{n-1}) + 4$, which can be written as $vol(T_n)+4 = 2(vol(T_{n-1})+4) = 2^2(vol(T_{n-2})+4) = \cdots = 2^{n-1}(vol(T_1)+4) = 2^{n+1}$. Therefore the volume of a tree is $vol(T_n) = 2^{n+1} - 4$ and the volume of a double tree is $vol(DT_n) = 2vol(T_n) + 2 = 2^{n+2} - 6$.*

   Let $A_1 = \{x(w) \mid w \in \Sigma^{\leq n}\}$ and $V \setminus A_1 = \{y(w) \mid w \in \Sigma^{\leq n}\}$. Then

$$\begin{aligned} vol(A_1) &= vol(T_n) + 1 \\ &= 2^{n+1} - 3, \\ vol(V \setminus A_1) &= 2^{n+1} - 3, \\ cut(A_1, V \setminus A_1) &= 1. \end{aligned}$$

   Therefore

$$\begin{aligned} Ncut(A_1, V \setminus A_1) &= \frac{2}{(vol(T_n)+1)} \\ &= \frac{2}{2^{n+1}-3} = \frac{4}{vol(DT_n)}. \end{aligned}$$

   Here $\kappa'(DT_n) = 1$ and $2vol(A_1) = vol(DT_n)$. Then from the Proposition 2.1, $Mcut(DT_n) = \dfrac{2}{2^{n+1}-3}$. ■

Next, we consider the graph $R_{n,k}$ and derive a formula for $Mcut(R_{n,k})$ based on n, k.

Proposition 2.4
For $R_{n,k}$ $(n \geq 1, k > 1)$, $Mcut(R_{n,k})$ is given by

$$\begin{cases} \frac{2}{3} & (n=1, k=2), \\ \frac{4}{-2+3k+2n} & (*_1 \wedge (k \geq 4) \wedge (n < K_1)), \\ \frac{4(-2+3k+2n)}{(-5+3k+2n)(1+3k+2n)} & (*_4 \wedge (k \geq 4) \wedge (n < K_4)), \\ \frac{4(-2+3k+2n)}{(-4+3k+2n)(3k+2n)} & (*_3 \wedge (k \geq 4) \wedge (n < K_3)), \\ \frac{4(-2+3k+2n)}{(-3+3k+2n)(-1+3k+2n)} & (*_2 \wedge (k \geq 4) \wedge (n < K_2)), \vee (n=1, k=3) \vee (n=2, k=3), \\ \frac{6k+4n-4}{(2n-1)(6k+2n-3)} & \begin{array}{c} ((k \geq 4) \wedge ((*_1 \wedge (K_1 \leq n)) \vee (*_4 \wedge (K_4 \leq n)) \vee \\ (*_3 \wedge (K_3 \leq n)) \vee (*_2 \wedge (K_2 \leq n)))) \vee \\ (k=2 \wedge (n \geq 2)) \vee (k=3 \wedge (n \geq 3)), \end{array} \end{cases}$$

where

$$\begin{aligned} *_1 &= ((2 \mid k) \wedge (3 \mid n)), \\ *_2 &= ((2 \nmid k) \wedge (3 \nmid n)), \\ *_3 &= ((2 \mid k) \wedge (3 \nmid n)), \\ *_4 &= ((2 \nmid k) \wedge (3 \mid n)), \\ K_1 &= 1 - \frac{1}{\sqrt{2}} - \frac{3k}{2} + \frac{3k}{\sqrt{2}}, \\ K_2 &= 1 - \frac{3k}{2} + \frac{\sqrt{1-12k+18k^2}}{2}, \\ K_3 &= 1 - \frac{3k}{2} + \frac{\sqrt{-1-6k+9k^2}}{\sqrt{2}}, \\ K_4 &= 1 - \frac{3k}{2} + \frac{\sqrt{-7-12k+18k^2}}{2}. \end{aligned}$$

(Proof) Let $V(R_{n,k}) = \{x_i \mid 1 \leq i \leq n+k\} \cup \{y_i \mid 1 \leq i \leq n+k\}$. Volume of $R_{n,k}$ is $vol(R_{n,k}) = 2(2n-1+3k-1) = 6k+4n-4$.
We consider the following cases in order to find the $Mcut(R_{n,k})$.
Case(i) *Let $A_1 \subseteq V(R_{n,k})$, where $A_1 = \{x_i \mid 1 \leq i \leq n+k\}$ and $V \setminus A_1 = \{y_i \mid 1 \leq i \leq n+k\}$. Then the volume $vol(A_1)$ is $\frac{vol(R_{n,k})}{2} = 2n+3k-2$ and $cut(A_1, V \setminus A_1) = k$. So we have*

$$\begin{aligned} Ncut(A_1, V \setminus A_1) &= k\left(\frac{1}{2n+3k-2} + \frac{1}{3k+2n-2}\right) \\ &= \frac{2k}{3k+2n-2}. \end{aligned}$$

Let this value as c_1.

Case(ii) *Let $A_2 \subseteq V(R_{n,k})$ such that $A_2 = \{x_i \mid 1 \leq i \leq n\}$ and $V \setminus A_2 = \{x_i \mid n+1 \leq i \leq n+k\} \cup \{y_i \mid 1 \leq i \leq n+k\}$. Then the volume $vol(A_2) = 2n-1$, $vol(V \setminus A_2) = vol(R_{n,k}) - vol(A_2) = 2n+6k-3$ and $cut(A_2, (V \setminus A_2)) = 1$. So we have*

$$Ncut(A_2, V \setminus A_2) = \frac{(6k+4n-4)}{(2n-1)(6k+2n-3)}.$$

Let this value as c_2.

Case(iii) *Suppose there exists $|A_3| < n$ such that $cut(A_3, (V \setminus A_3)) = 1$. Let $vol(A_3) = 2n-1-2x$ where $x = |A_2| - |A_3|$ where $|A_2| = n$. Then $vol(V \setminus A_3) = 6k+2n-3+2x$. $Ncut(A_3, V \setminus A_3) = \frac{1}{2n-1-2x} + \frac{1}{6k+2n-3+2x} = \frac{6k+4n-4}{(2n-1)(6k+2n-3)+4x(1-(3k+x))}$. Since $4x(1-(3k+x)) < 0$, $Ncut(A_3, V \setminus A_3) > Ncut(A_2, V \setminus A_2)(Case(ii) < Case(iii))$. Since c_2 is smaller than $Case(iii)$ we can ignore this case.*

Case(iv)*Let $A_4 = \{x_i \mid 1 \leq i \leq n+\alpha\} \cup \{y_i \mid 1 \leq i \leq n+\alpha\}$, where $1 \leq \alpha < k$ and $V \setminus A_4 = \{x_i \mid n+\alpha+1 \leq i \leq n+k\} \cup \{y_i \mid n+\alpha+1 \leq i \leq n+k\}$. Then $vol(A_4) = 2(2n-1+3\alpha) = 4n+6\alpha-2$, $vol(V \setminus A_4) = 6k-2-6\alpha$ and $cut(A_4, V \setminus A_4) = 2$. Then we have,*

$$Ncut(A_4, V \setminus A_4) = \frac{(3k+2n-2)}{(2n-1+3\alpha)(3k-3\alpha-1)}.$$

Let this value as $c_4(\alpha)$.

Minimum of $c_4(\alpha)$ can be obtained by differentiating with respect to α.

$\frac{dc_4(\alpha)}{d\alpha} = 0$ *gives minimum value of $c_4(\alpha)$ at $\alpha_0 = \frac{3k-2n}{6}$. But α_0 is not an integer for all n, k.*

If $\frac{3k-2n}{6} < 1$ that is $1 \leq k < \frac{6+2n}{3}$ then the minimum value is $c_4(1)$. Then we have

$$c_4(1) = \frac{2-3k-2n}{8-6k+8n-6kn}.$$

If $1 \leq \frac{3k-2n}{6} < k$ that is $k \geq \frac{6+2n}{3}$ then the minimum value is $c_4(\frac{3k-2n}{6})$ whenever $\frac{3k-2n}{6} \in$ $\mathbf{Z}$.

$$c_4(\frac{3k-2n}{6}) = \frac{4}{-2+3k+2n}.$$

If $k \geq \frac{6+2n}{3}$ and $2 \nmid k$ and $3 \mid n$ then the minimum value is $c_4(\frac{3k-2n}{6} + \frac{1}{2}) = c_4(\frac{3k-2n}{6} - \frac{1}{2})$.

$$c_4(\frac{3k-2n}{6} + \frac{1}{2}) = \frac{4(-2+3k+2n)}{(-5+3k+2n)(1+3k+2n)}.$$

If $k \geq \frac{6+2n}{3}$ and $3 \nmid n$ and $2 \mid k$ then the minimum value is $c_4(\frac{3k-2n}{6} + \frac{1}{3}) = c_4(\frac{3k-2n}{6} - \frac{1}{3})$.

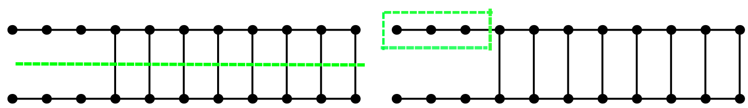
$$c_4(\frac{3k-2n}{6} - \frac{1}{3}) = \frac{4(-2+3k+2n)}{(-4+3k+2n)(3k+2n)}.$$

If $k \geq \frac{6+2n}{3}$ and $3 \nmid n$ and $2 \nmid k$ then the minimum value is $c_4(\dfrac{3k-2n}{6} + \dfrac{1}{6}) = c_4(\dfrac{3k-2n}{6} - \dfrac{1}{6})$.

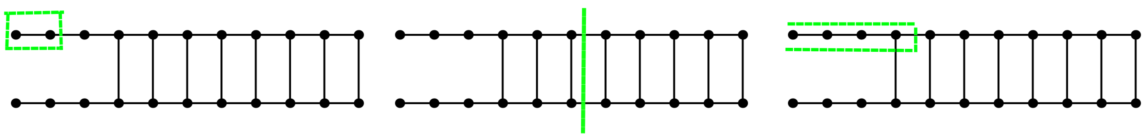
$$c_4(\frac{3k-2n}{6} - \frac{1}{6}) = \frac{4(-2+3k+2n)}{(-3+3k+2n)(-1+3k+2n)}.$$

Case(v) *Let $A_5 = \{x_i \mid 1 \leq i \leq n+1\}$ and $V \setminus A_5 = \{x_i \mid n+2 \leq i \leq n+k\} \cup \{y_i \mid 1 \leq i \leq n+k\}$. Then $vol(A_5) = 2n+2$ and $vol(V \setminus A_5) = 2n+6k-6$. Then we have $Ncut(A_5, V \setminus A_5) = 2\left(\dfrac{1}{2n+2} + \dfrac{1}{2n+6k-6}\right) = \dfrac{2n+3k-2}{(n+1)(n+3k-3)}$.*

Figure 6 shows the partitions appeared in Case(i) to Case(v).



(a) *Case(i)* (b) *Case(ii)*



(c) *Case(iii)* (d) *Case(iv)* (e) *Case(v)*

Figure 6: Partitions of $R_{n,k}$.

Now we can compare all cases considered above.
If $k = 2$ and $n = 1$ then it is easy show that c_1 is the minimum. If $k = 2$ and $n \geq 2$ then it is easy to show that c_2 is the minimum. If $k = 3$ and $n = 1$ then $c_4(\frac{3k-2n}{6} - \frac{1}{6})$ is the minimum. If $k = 3$ and $n = 2$ then $c_4(\frac{3k-2n}{6} + \frac{1}{6})$ is the minimum. If $k = 3$ and $n \geq 3$ then we can easily show that c_2 is the minimum. If $k \geq 4$ and $n = 1$ then c_4 is the minimum. Next we assume that $k \geq 4$ and $n \geq 2$. It is easy to check that c_2 is smaller than c_1, c_3 and c_5. So we compare c_2 with c_4 for $k \geq 4$. Then we have

the following results. If $(*_1$ *and* $(n < K_1))$ *then* $c_4(\frac{3k-2n}{6})$ *is smaller than* c_2*. If* $(*_2$ *and* $(n < K_2))$ *then* $c_4(\frac{3k-2n}{6} - \frac{1}{6})$ *is smaller than* c_2*. If* $(*_3$ *and* $(n < K_3))$ *then* $c_4(\frac{3k-2n}{6} - \frac{1}{3})$ *is smaller than* c_2*. If* $(*_4$ *and* $(n < K_4))$ *then* $c_4(\frac{3k-2n}{6} + \frac{1}{2})$ *is smaller than* c_2*. We can summarize the results as follows.*

$$\begin{cases} c_1 & n = 1, k = 2, \\ c_4(\frac{3k-2n}{6}) & (*_1 \wedge (k \geq 4) \wedge (n < K_1)), \\ c_4(\frac{3k-2n}{6} + 1/2) & (*_4 \wedge (k \geq 4) \wedge (n < K_4)), \\ c_4(\frac{3k-2n}{6} - 1/3) & (*_3 \wedge (k \geq 4) \wedge (n < K_3)), \\ c_4(\frac{3k-2n}{6} - 1/6) & (*_2 \wedge (k \geq 4) \wedge (n < K_2)) \vee (n = 1, k = 3) \vee (n = 2, k = 3), \\ c_2 & ((k \geq 4) \wedge ((*_1 \wedge (K_1 \leq n)) \vee (*_2 \wedge (K_2 \leq n)))) \\ & \vee (*_3 \wedge (K_3 \leq n)) \vee (*_4 \wedge (K_4 \leq n)) \\ & \vee (k = 2 \wedge (n \geq 2)) \vee (k = 3 \wedge (n \geq 3)). \end{cases}$$

Finally, we want to show that for any arbitrary subset A*,* $cut(A, V \setminus A) = 1$ *or* $cut(A, V \setminus A) = 2$ *gives the minimum normalized cut. We notice that every subset* A *with* $cut(A, V \setminus A) = 1$ *is* A_2 *or* A_3 *and every subset* A *with* $cut(A, V \setminus A) = 2$ *are* A_1, A_5, A_4*. We consider all cases with* $cut(A, V \setminus A) = 1$ *and the minimum occurs at* A_2*. There may be several partitions with* $cut(A, V \setminus A) \geq 2$*. Let* $k \geq 4$*. Then we note that* $vol(R_{n,k}) \geq 24$ *and there exists a subset* A_4 *in Case(iv), which minimize the* $\left(\frac{1}{vol(A)} + \frac{1}{vol(G) - vol(A)}\right)$ *with* $cut(A, V \setminus A) = 2$*. We note that* $|vol(A_4) - \frac{vol(G)}{2}| \leq 3$*. From Lemma 2.3,* $3\left(\frac{1}{vol(G)/2} + \frac{1}{vol(G)/2}\right) > 2\left(\frac{1}{vol(G)/2 + 3} + \frac{1}{vol(G)/2 - 3}\right)$ *for* $vol(G) \geq 11$*. Then we can show that there is no subset* A *with* $cut(A, V \setminus A) \geq 3$ *and* $Mcut(A, V \setminus A) \leq Mcut(A_4, V \setminus A_4)$*. This conclude that minimum Ncut always have cut value 2 for all cases which has cut size more than 1.* ■

The Figure 7 shows the above regions for n, k*. For a given* n *and* k*, we can find* $Mcut(R_{n,k})$*.*

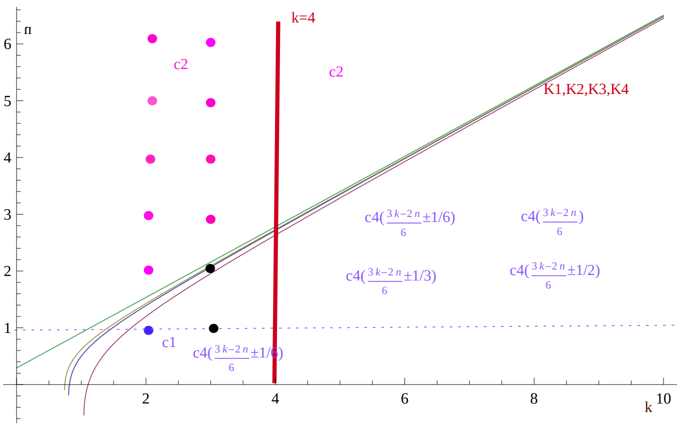


Figure 7: $Mcut(R_{n,k})$.

2.4 $Mcut$ of weighted paths $P_{n,k}$

In this section, we consider a weighted path graph $P_{n,k}$ and find a formula for $Mcut(P_{n,k})$ based on n, k.

Proposition 2.5
For $P_{n,k}, (n, k \geq 1)$, $Mcut(P_{n,k})$ is given by

$$\begin{cases} \frac{4}{-2+3k+2n} & ((o_1 \wedge (k \geq R_3)) \vee ((k < R_1) \wedge (o_4 \in \mathbf{Z})) \vee (n=1, k=1)), \\ \frac{4(-2+3k+2n)}{(-5+3k+2n)(1+3k+2n)} & (o_2 \wedge (k \geq R_3)), \\ \frac{4(-2+3k+2n)}{(-4+3k+2n)(3k+2n)} & (o_3 \wedge (k \geq R_3)) \vee (((k < R_1) \wedge (o_4 \notin \mathbf{Z})) \wedge (2 \mid k)), \\ \frac{4(-2+3k+2n)}{(-3+3k+2n)(-1+3k+2n)} & (2 \nmid k) \wedge ((k < R_1) \vee (k \geq R_3)), \\ \frac{3k+2n-2}{(3k-4)(2n+2)} & ((n > 2) \wedge (R_2 \leq k < R_3)) \vee (n=1, k=2) \vee (n=2, k=3), \\ \frac{3k+2n-2}{(3k-1)(2n-1)} & (n \geq 2 \wedge (R_1 \leq k \leq R_2)), \end{cases}$$

where

$$\begin{aligned} o_1 &= ((3 \mid n) \wedge (2 \mid k)), \\ o_2 &= ((3 \mid n) \wedge (2 \nmid k)), \\ o_3 &= ((3 \nmid n) \wedge (2 \mid k)), \\ o_4 &= \frac{3k+2n}{4}, \\ R_1 &= \frac{2n}{3}, \\ R_2 &= \frac{2n}{3} + 1, \\ R_3 &= \frac{2n}{3} + 2. \end{aligned}$$

(Proof) Let $P_{n,k}$ be a weighted graph such that $E(P_{n,k}) = \{(x_i, x_{i+1}) \mid 1 \leq i \leq n+k-1\}$ and $V(P_{n,k}) = \{x_i \mid 1 \leq i \leq n+k\}$.
We consider the following cases to find the $Mcut(P_{n,k})$.

Case(i) *Let $A_1 \subseteq V(P_{n,k})$, where $A_1 = \{x_i \mid 1 \leq i \leq n\}$ and $V \setminus A_1 = \{x_i \mid n+1 \leq i \leq k\}$. Then the volume $vol(A_1)$ is $2n-1$ and $cut(A_1, V \setminus A_1) = 1$. So we have*

$$Ncut(A_1, V \setminus A_1) = \frac{1}{2n-1} + \frac{1}{3k-1} = \frac{3k+2n-2}{(2n-1)(3k-1)},$$

and let this value as c_1.

Case(ii) *Let* $A_2 = \{x_i \mid 1 \leq i \leq \alpha\}(1 \leq \alpha < n)$ *and* $V \setminus A_2 = \{x_i \mid \alpha+1 \leq i \leq n+k\}$. *Then*

$$Ncut(A_2, V \setminus A_2) = \frac{1}{2\alpha - 1} + \frac{1}{3k - 1 + 2(n - \alpha)},$$

and let this value as $c_2(\alpha)$.

Minimum of $c_2(\alpha)$ *can be obtained by differentiating with respect to* α. $\frac{dc_2(\alpha)}{d\alpha} = 0$ *gives the minimum value for* α *and let this value as* $\alpha_0 = \frac{3k+2n}{4}$. *But* α_0 *is not an integer value for all* n, k. *So we consider several cases here.*

If $\frac{3k+2n}{4} < n$ *that is* $k < \frac{2n}{3}$, *the minimum value is* $c_2(\frac{3k+2n}{4})$, *whenever* $\frac{3k+2n}{4}$ *is an integer.*

$$c_2(\frac{3k+2n}{4}) = \frac{4}{-2+3k+2n}.$$

If $k < \frac{2n}{3}$ *and* $\frac{3k+2n}{4} \notin \mathbf{Z}$ *and* $2 \mid k$ *then the minimum value is* $c_2(\frac{3k+2n}{4} \pm \frac{1}{2})$. *We note that* $c_2(\frac{3k+2n}{4} + \frac{1}{2}) = c_2(\frac{3k+2n}{4} - \frac{1}{2})$. *Then we have,*

$$c_2(\frac{3k+2n}{4} + \frac{1}{2}) = \frac{4(-2+3k+2n)}{(-4+3k+2n)(3k+2n)}.$$

If $k < \frac{2n}{3}$ *and* $\frac{3k+2n}{4} \notin \mathbf{Z}$ *and* $2 \nmid k$ *then the minimum value is* $c_2(\frac{3k+2n}{4} \pm \frac{1}{4})$. *We note that* $c_2(\frac{3k+2n}{4} + \frac{1}{4}) = c_2(\frac{3k+2n}{4} - \frac{1}{4})$. *Then we have,*

$$c_2(\frac{3k+2n}{4} + \frac{1}{4}) = \frac{4(-2+3k+2n)}{(-3+3k+2n)(-1+3k+2n)}.$$

If $\frac{3k+2n}{4} \geq n$ *that is* $k \geq \frac{2n}{3}$, *the minimum value is* $c_2(n)$. *This is equal to the Case(i).*

$$c_2(n) = \frac{3k+2n-2}{(3k-1)(2n-1)}.$$

Case(iii) *Let* $A_3 = \{x_i \mid 1 \leq i \leq \alpha\}$, *where* $n+1 \leq \alpha < n+k$ *and* $V \setminus A_3 = \{x_i \mid \alpha+1 \leq i \leq n+k\}$. *Then* $vol(A_3) = 2n - 1 + 3(\alpha - n)$ *and* $vol(V \setminus A_3) = 3k - 1 - 3(\alpha - n)$. *Since* $cut(A_3, V \setminus A_3) = 1$,

$$Ncut(A_3, V \setminus A_3) = \frac{3k+3n-2}{(-1+3\alpha-n)(3k-1-3\alpha+3n)},$$

and let this value as $c_3(\alpha)$.

Minimum of Case(iii) can be obtained by differentiating with respect to α. $\frac{dc_3(\alpha)}{d\alpha} = 0$ *gives the minimum value at* $\alpha_1 = \frac{3k+4n}{6}$. *But this value is not an integer for all* n, k. *So we consider several cases here.*

If $n+1 \leq \dfrac{3k+4n}{6} < n+k$ *that is* $k \geq \dfrac{6+2n}{3}$*, the minimum value is* $c_3(\dfrac{3k+4n}{6})$ *whenever* $\dfrac{3k+4n}{6}$ *is an integer. Then we have*

$$c_3(\frac{3k+4n}{6}) = \frac{4}{-2+3k+2n}.$$

If $k \geq \dfrac{6+2n}{3}$ *and* $2 \nmid k$ *and* $3 \mid n$ *then the minimum value is* $c_3(\dfrac{3k+4n}{6}+\dfrac{1}{2}) = c_3(\dfrac{3k+4n}{6}-\dfrac{1}{2})$. *Then we have*

$$c_3(\frac{3k+4n}{6}+\frac{1}{2}) = \frac{4(-2+3k+2n)}{(-5+3k+2n)(1+3k+2n)}.$$

If $k \geq \dfrac{6+2n}{3}$ *and* $3 \nmid n$ *and* $2 \mid k$*, then the minimum value is* $c_3(\dfrac{3k+4n}{6}+\dfrac{1}{3}) = c_3(\dfrac{3k+4n}{6}-\dfrac{1}{3})$. *Then we have,*

$$c_3(\frac{3k+4n}{6}-\frac{1}{3}) = \frac{4(-2+3k+2n)}{(-4+3k+2n)(3k+2n)}.$$

If $k \geq \dfrac{6+2n}{3}$*, and* $2 \nmid k$*, then the minimum value is* $c_3(\dfrac{3k+4n}{6}+\dfrac{1}{6}) = c_3(\dfrac{3k+4n}{6}-\dfrac{1}{6})$*. Then we have,*

$$c_3(\frac{3k+4n}{6}+\frac{1}{6}) = \frac{4(-2+3k+2n)}{(-3+3k+2n)(-1+3k+2n)}.$$

Similarly, for $\dfrac{3k+4n}{6} < n+1$ *that is for* $k < \dfrac{6+2n}{4}$*, the minimum value is* $c_3(n+1)$.

$$c_3(n+1) = \frac{3k+2n-2}{(3k-4)(2n+2)}.$$

Now we can compare all cases considered above.
Compare $c_3(\frac{3k+4n}{6})$, $c_3(\frac{3k+4n}{6}+\frac{1}{2})$, $c_3(\frac{3k+4n}{6}-\frac{1}{3})$ *and* $c_3(\frac{3k+4n}{6}+\frac{1}{6})$ *with* $c_2(n)$*, for* $k \geq R_3$. $c_3(\frac{3k+4n}{6})$, $c_3(\frac{3k+4n}{6}+\frac{1}{2})$, $c_3(\frac{3k+4n}{6}-\frac{1}{3})$ *and* $c_3(\frac{3k+4n}{6}+\frac{1}{6})$ *are smaller than* $c_2(n)$ *for* $k \geq R_3$*. Now compare* $c_2(\frac{3k+2n}{4})$, $c_2(\frac{3k+2n}{4}+\frac{1}{2})$ *and* $c_2(\frac{3k+2n}{4}+\frac{1}{4})$ *with* $c_3(n+1)$ *for* $k < R_1$*. This case holds when* $n > \dfrac{3}{2}$ *and* $1 \leq k < R_1$*. That is for* $n > 1$ *and* $1 \leq k < R_1$*. In this region,* $c_2(\dfrac{3k+2n}{4})$, $c_2(\dfrac{3k+2n}{4}+\dfrac{1}{2})$ *and* $c_2(\dfrac{3k+2n}{4}+\dfrac{1}{4})$ *is smaller than* $c_3(n+1)$*. Finally compare* $c_2(n)$ *with* $c_3(n+1)$ *for* $k < R_3$ *and* $k \geq R_1$*. Then* $c_3(n+1)$ *is smaller than* $c_2(n)$ *when* $(n=1, k=2)$ *and* $(n=2, k=3)$ *and* $((n>2) \wedge (R_2 \leq k < R_3))$. $c_2(n)$ *is smaller than* $c_3(n+1)$ *when* $(n=2, k=2)$ *and* $((n>2) \wedge (R_1 \leq$

$k \leq R_2)$). *So we obtain the following results for* $Mcut(P_{n,k})$.

$$\begin{cases} c_3(\frac{3k+4n}{6}) & ((k \geq R_3) \wedge o_1) \vee (n=1, k=1), \\ c_3(\frac{3k+4n}{6}+\frac{1}{2}) & ((k \geq R_3) \wedge o_2), \\ c_3(\frac{3k+4n}{6}-\frac{1}{3}) & ((k \geq R_3) \wedge o_3), \\ c_3(\frac{3k+4n}{6}+\frac{1}{6}) & ((k \geq R_3) \wedge (2 \nmid k)), \\ c_3(n+1) & ((n>2) \wedge (R_2 \leq k < R_3)) \vee (n=1, k=2) \vee (n=2, k=3), \\ c_2(n) & ((n>2) \wedge (R_1 \leq k \leq R_2)) \vee (n=2, k=2), \\ c_2(\frac{3k+2n}{4}) & (k < R_1) \wedge (o_4 \in \mathbf{Z}), \\ c_2(\frac{3k+2n}{4}+\frac{1}{2}) & ((k < R_1) \wedge (o_4 \notin \mathbf{Z}) \wedge (2 \mid k)), \\ c_2(\frac{3k+2n}{4}+\frac{1}{4}) & ((k < R_1) \wedge (o_4 \notin \mathbf{Z}) \wedge (2 \nmid k)). \end{cases}$$

The Figure 8 shows the minimum $Mcut(P_{n,k})$ *for each* n, k.

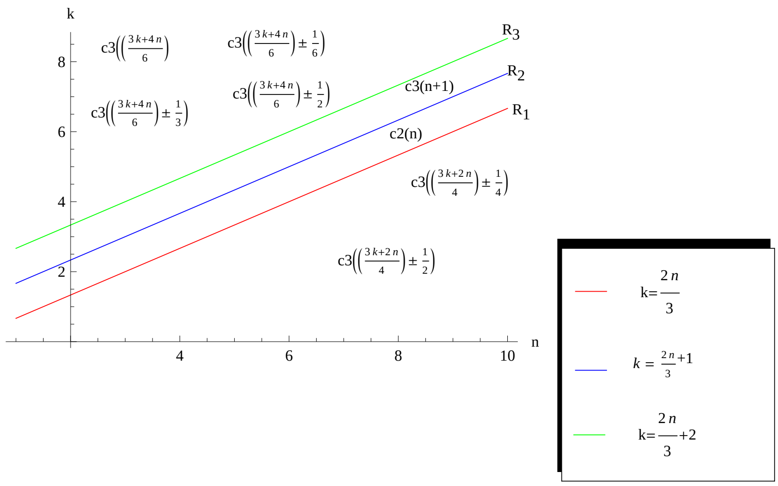


Figure 8: $Mcut(P_{n,k})$.

$\blacksquare$

Corollary 2.1
For $P_{2k,k} (k \geq 1)$,

$$Mcut(P_{2k,k}) = \begin{cases} \frac{4}{-2+7k} & (4 \mid k), \\ \frac{4(-2+7k)}{(-4+7k)(7k)} & (4 \nmid k) \wedge (2 \mid k), \\ \frac{4(-2+7k)}{(-3+7k)(-1+7k)} & (2 \nmid k). \end{cases}$$

(Proof) By substituting $n = 2k$ *to the formula given for* $Mcut(P_{n,k})$, *we can directly obtain the result. According to the Proposition 2.5, for* $n = 2k$, $k \geq \dfrac{2n}{3} + 2$ *implies that* $k \leq -6$. *Since* $k \geq 1$, *this does*

not holds. For $n = 2k$, $\frac{2n}{3} \le k < \frac{2n}{3} + 2$ *implies that* $-2 < k < 0$. *Since* $k \ge 1$, *this does not holds. Therefore the only case, which holds for* $n = 2k$ *is,* $k < \frac{4k}{3}$. *That is* $k \le R_2$ *in the Proposition 2.5. This implies that* $k > 0$. *Substituting* $n = 2k$ *in the Proposition 2.5, we have,*

$$Mcut(P_{2k,k}) = \begin{cases} \frac{4}{-2+7k} & (4 \mid k), \\ \frac{4(-2+7k)}{(-4+7k)(7k)} & (4 \nmid k) \wedge (2 \mid k), \\ \frac{4(-2+7k)}{(-3+7k)(-1+7k)} & (2 \nmid k). \end{cases}$$

■

2.5 $Mcut$ of graph $LP_{n,m}$

Here, we consider the lollipop graph $LP_{n,m}$ *and derive a formula for* $Mcut(LP_{n,m})$. *As defined in the preliminary section, lollipop graph* $LP_{n,m}$ *is constructed by joining the end vertex of a path graph* P_m *to the vertex of a complete graph* K_n.

Proposition 2.6
For the graph $LP_{n,m}$, ($n \ge 3$ and $m \ge 1$),

$$Mcut(LP_{n,m}) = \begin{cases} \frac{n^2-n+2m}{(n^2-n+1)(2m-1)} & 2 \le m \le \frac{n^2-n+4}{2}, \\ \frac{4}{(n^2-n+2m)} & \frac{n^2-n+2m+2}{4} \in \mathbf{Z} \wedge m > \frac{n^2-n+4}{2}, \\ \frac{4(2m+(-1+n)n)}{-4+4m^2+4m(-1+n)n+n^2-2n^3+n^4} & \frac{n^2-n+2m+2}{4} \notin \mathbf{Z} \wedge m > \frac{n^2-n+4}{2}, \\ \frac{n^2-n+2}{(n^2-1)} & m = 1. \end{cases}$$

(Proof) Let $V(LP_{n,m}) = \{x_1, x_2, \ldots, x_m, y_1, y_2, \ldots, y_n\}$, *where the set of vertices* $\{x_1, x_2, \ldots, x_m\} = V(P_m)$ *and* $\{y_1, y_2, \ldots, y_n\} = V(K_n)$. *Let* $E(LP_{n,m}) = \{(x_i, x_{i+1}) \mid 1 \le i \le m-1\} \cup \{(y_i, y_j) \mid 1 \le i, j \le n$ *and* $i \ne j\} \cup \{(y_1, x_m)\}$. *We consider the following cases by taking subsets from the graph.*
Case(i) *Let* $A_1 \subset V(LP_{n,m})$ *such that* $A_1 = \{x_i \mid 1 \le i \le m\}$ *and* $V \setminus A_1 = \{y_i \mid 1 \le i \le n\}$. *Then* $cut(A_1, V \setminus A_1) = 1$. $vol(A_1) = vol(P_m) + 1 = 2m - 1$. $vol(V \setminus A_1) = vol(K_n) + 1 = n(n-1) + 1$. *Then* $Ncut(A_1, V \setminus A_1) = \frac{1}{2m-1} + \frac{1}{n^2-n+1} = \frac{n^2-n+2m}{(n^2-n+1)(2m-1)}$. *Let this value as* c_1.
Case(ii) *Let* $A_2 \subset V(LP_{n,m})$ *such that* $A_2 = \{x_i \mid 1 \le i \le m\} \cup \{y_1\}$ *and* $V \setminus A_2 = \{y_i \mid 2 \le i \le n\}$. *Then* $cut(A_2, V \setminus A_2) = n-1$, $vol(A_2) = vol(P_m)+1+n = 2m-1+n$ *and* $vol(V \setminus A_2) = n(n-1)+1-n = (n-1)^2$. *Then* $Ncut(A_2, V \setminus A_2) = (n-1)\left(\frac{1}{2m-1+n} + \frac{1}{(n-1)^2}\right) = \frac{n^2-n+2m}{(n-1)(2m-1+n)} (n \ne 1)$. *Let this value as* c_2.

Case(iii) *Let* $A_3 \subset V(LP_{n,m})$ *such that* $A_3 = \{x_i \mid 1 \le i \le k\}$ *and* $V \setminus A_3 = \{y_i \mid 1 \le i \le n\} \cup \{x_i \mid k+1 \le i \le m\}$. *Then* $cut(A_3, V \setminus A_3) = 1$, $vol(A_3) = vol(P_k) + 1 = 2k - 1$ *and* $vol(V \setminus A_3) = vol(K_n) + 1 + vol(P_m) - vol(P_k) = n(n-1) + 1 + 2(m-k)$. *Then* $Ncut(A_3, V \setminus A_3) = \frac{1}{2k-1} + \frac{1}{n(n-1)+1+2(m-k)} = \frac{n^2-n+2m}{(n(n-1)+1+2(m-k))(2k-1)}$. *Let this value as* $c_3(k)$. *We can find the minimum value of* c_3 *by differentiating* $c_3(k)$ *with respect to* k. $\frac{dc_3(k)}{dk} = 0$ *gives*

$k_0 = \dfrac{n^2-n+2m+2}{4}$. *If* $1 \le \dfrac{n^2-n+2m+2}{4} < m$ *for* $m \ge 1, n \ge 3$, *that is* $m > \dfrac{2-n+n^2}{2}$ *then the minimum of* $c_3(k)$ *is* $c_3(k_0)$ *whenever* $k_0 = \dfrac{n^2-n+2m+2}{4} \in \mathbf{Z}$. *Then we have,*

$$c_3(k_0) = \frac{4}{2m+n^2-n}.$$

If $k_0 \notin \mathbf{Z}$ *then let* k_0 *as* $k_0 = \dfrac{n^2-n+2m+2}{4} \pm \dfrac{1}{2}$. *If* $k = \dfrac{n^2-n+2m+2}{4} + \dfrac{1}{2}$ *then the minimum of* $c_3(k)$ *is given by*

$$c_3(k_0+\frac{1}{2}) = \frac{4(2m-n+n^2)}{(-2+2m-n+n^2)\,(2+2m-n+n^2)}.$$

If we let k_0 *as* $k_0 = \dfrac{n^2-n+2m+2}{4} - \dfrac{1}{2}$ *then the minimum of* c_3 *is*

$$c_3(k_0-\frac{1}{2}) = \frac{4(2m-n+n^2)}{(-2+2m-n+n^2)\,(2+2m-n+n^2)}.$$

So we have $c_3(k_0-\dfrac{1}{2}) = c_3(k_0+\dfrac{1}{2}) = \dfrac{4(2m-n+n^2)}{(-2+2m-n+n^2)\,(2+2m-n+n^2)}$.

If $\dfrac{n^2-n+2m+2}{4} \ge m$ *that is* $m \le \dfrac{2-n+n^2}{2}$ *then the minimum of* $c_3(k)$ *is* $c_3(m)$. *This is equal to the Case(i) considered above. Hence for* $m \le \dfrac{2-n+n^2}{2}$, *we have*

$$c_3(m) = \frac{n^2-n+2m}{(n^2-n+1)(2m-1)}.$$

Case(iv) *Let* $A_4 \subset V(LP_{n,m})$ *such that* $A_4 = \{x_i \mid 1 \le i \le m\} \cup \{y_i \mid 1 \le i \le k \text{ and } j+1 \le i \le n\}$ *and* $V \setminus A_4 = \{y_i \mid k+1 \le i \le j\}$, *where* $|V \setminus A_4| = \lfloor \dfrac{n}{2} \rfloor$. *Then* $cut(A_4, V \setminus A_4) = \lfloor \dfrac{n}{2} \rfloor \lceil \dfrac{n}{2} \rceil$. *Volume of* $vol(A_4) = 2m - 1 + \lceil \dfrac{n}{2} \rceil (n-1) + 1$. *Volume of* $vol(V \setminus A_4) = \lfloor \dfrac{n}{2} \rfloor (n-1)$. *Then* $Ncut(A_4, V \setminus A_4) = \dfrac{\lceil \frac{n}{2} \rceil \lfloor \frac{n}{2} \rfloor (n(n-1)+2m)}{2m(n-1)\lfloor \frac{n}{2} \rfloor + \lceil \frac{n}{2} \rceil \lfloor \frac{n}{2} \rfloor (n-1)^2}$. *This can be written as,*

$$\begin{cases} \frac{n^2(n(n-1)+2m)}{(4m+n^2-1)(n(n-1))} & \text{if } n \text{ is even,} \\ \frac{n^2(n(n-1)+2m)}{(4m+n^2-1)(n-1)^2} & \text{if } n \text{ is odd.} \end{cases}$$

Let this value as c_4. *Now we can compare all cases considered above. Comparing* c_4 *with* c_1, c_1 *is the minimum for* $n \ge 3$ *and* $m \ge 1$. *Next we compare value of* $c_3(k_0), c_3(k_0+\frac{1}{2})$ *with* c_2 *in the region* $m > \dfrac{2-n+n^2}{2}$. $c_3(k_0)$ *and* $c_3(k_0+\frac{1}{2})$ *are smaller than* c_2. *Next compare* $c_3(m)$ *with* c_2 *for* $m \le \dfrac{2-n+n^2}{2}$. *Then for* $2 \le m \le \dfrac{2-n+n^2}{2}$, $c_3(m)$ *is smaller than* c_2.
When $m = 1$,

$$c_2 = \frac{n^2-n+2}{(n^2-1)}.$$

In this case, c_2 *is smaller than* $c_3(m)$.

Hence we can summarize the results as follows.

$$Mcut(LP_{n,m}) = \begin{cases} c_3(m) & 2 \leq m \leq \frac{n^2-n+2}{2}, \\ c_3(k_0) & k_0 \in \mathbf{Z} \text{ and } m > \frac{n^2-n+2}{2}, \\ c_3(k_0+\frac{1}{2}) & k_0 \notin \mathbf{Z} \text{ and } m > \frac{n^2-n+2}{2}, \\ c_2 & m = 1. \end{cases}$$

The Figure 9 shows the values of $Mcut(LP_{n,m})$ *for each* n, m. ■

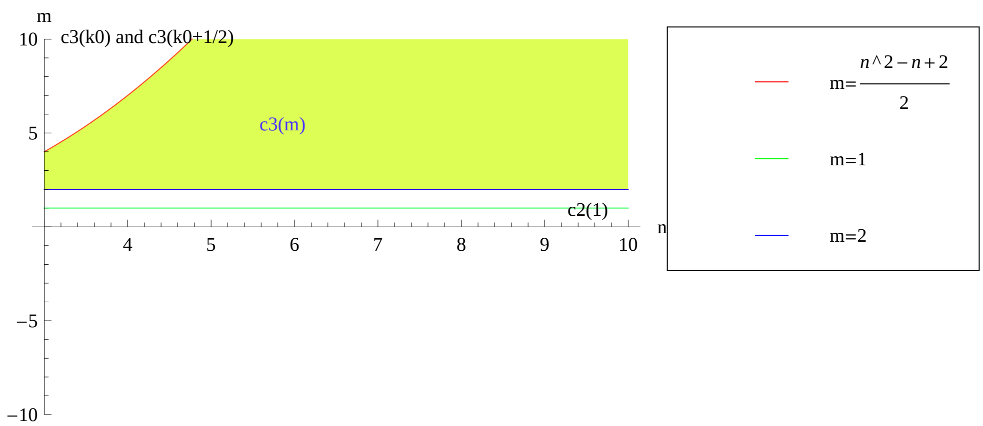


Figure 9: $Mcut(LP_{n,m})$.

2.6 $Mcut$ of graph $LP'_{n,2}$

In this section, we explain another graph, which we call $LP'_{n,2}$. *As explained in the preliminary section, we construct* $LP'_{n,2}$ *by joining both end vertices of path graph* P_2 *to the two adjacent vertices of complete graph* K_n.

Proposition 2.7
For the graph $LP'_{n,2}$, $Mcut(LP'_{n,2}) = \dfrac{n^2-n+6}{2(n^2-n+2)}$ *for* $n \geq 3$.

(Proof) Let $V(LP'_{n,2}) = \{x_1, x_2, y_1, y_2, \ldots, y_n\}$, *where* $\{x_1, x_2\} = V(P_2)$ *and* $\{y_1, y_2, \ldots, y_n\} = V(K_n)$. *Let* $E(G) = \{(x_1, x_2)\} \cup \{(y_i, y_j) \mid 1 \leq i \leq n, 1 \leq j \leq n \text{ and } i \neq j\} \cup \{(y_1, x_2)\} \cup \{(y_n, x_1)\}$. *Now consider the following cases.*
Case(i) *Let* $A_1 \subset V(LP'_{n,2})$ *such that* $A_1 = \{x_i \mid 1 \leq i \leq 2\}$ *and* $V \setminus A_1 = \{y_i \mid 1 \leq i \leq n\}$. *Then* $cut(A_1, V \setminus A_1) = 2, vol(A_1) = 4$ *and* $vol(V \setminus A_1) = n(n-1)+2$. *So we have* $Ncut(A_1, V \setminus A_1) = 2\left(\dfrac{1}{4} + \dfrac{1}{n(n-1)+2}\right) = \dfrac{n^2-n+6}{2(n^2-n+2)}$.

Case(ii) *Let* $A_2 \subset V(LP'_{n,2})$ *such that* $A_2 = \{x_2\} \cup \{y_i \mid 1 \leq i \leq \lfloor \frac{n}{2} \rfloor\}$ *and* $V \setminus A_2 = \{x_1\} \cup \{y_i \mid \lfloor \frac{n}{2} \rfloor + 1 \leq i \leq n\}$. *Then* $cut(A_2, V \setminus A_2) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + 1$ *and* $Ncut(A_2, V \setminus A_2) = (\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + 1) \left(\frac{1}{((n-1)\lfloor \frac{n}{2} \rfloor + 3)} + \frac{1}{((n-1)\lceil \frac{n}{2} \rceil + 3)} \right) = \frac{(\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + 1)((n-1)n+6)}{(n-1)^2 \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + 3(n-1)n + 9}$.
We can deduce this as

$$\begin{cases} \frac{4+n^2}{6-n+n^2} & n \text{ even}, \\ \frac{(3+n^2)(6-n+n^2)}{(5+n^2)(7-2n+n^2)} & n \text{ odd}. \end{cases}$$

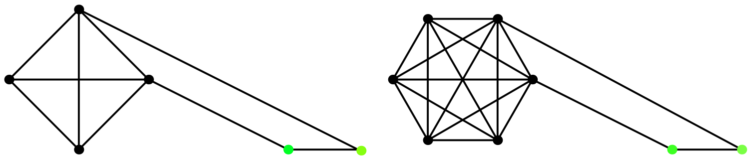
For even n, $Case(ii) - Case(i)$ *is* $\frac{(n^4 - n^2 + 4n - 20)}{2(n^2 - n + 2)(n^2 - n + 6)} > 0$ *for* $n \geq 3$. *For odd n,* $Case(ii) - Case(i) = \frac{(n^2 - n + 6)(n^4 - 2n^2 + 4n - 23)}{2(5 + n^2)(n^2 - 2n + 7)(n^2 - n + 2)} > 0$ *for* $n \geq 3$. *Hence* $Case(i) < Case(ii)$.
Case(iii) *Let* $A_3 \subset V(LP'_{n,2})$ *such that* $A_3 = \{x_1, x_2, y_1, y_n\}$ *and* $V \setminus A_3 = \{y_2, \ldots, y_{n-1}\}$. *Then* $cut(A_3, V \setminus A_3) = 2(n-2)$ *and* $Ncut(A_3, V \setminus A_3) = 2(n-2)(\frac{1}{4+2n} + \frac{1}{(n-2)(n-1)}) = \frac{n^2 - n + 6}{(n+2)(n-1)}$.
Now compare Case(iii) with Case(i). $Case(iii) - Case(i) = \frac{(n^2 - 3n + 6)(n^2 - n + 6)}{2(n+2)(n-1)(n^2 - n + 2)} > 0$. *Then Case(i) is the minimum.*
Case(iv) *Further we can consider a cut through the complete graph such that half of the complete graph belongs to one partition. Let* $A_4 = \{y_i \mid k \leq i \leq j\}$ *such that* $|A_4| = \lfloor \frac{n}{2} \rfloor$ *and* $(V \setminus A_4) = \{y_1, y_n\} \cup \{x_1, x_2\} \cup \{y_i \mid 1 \leq i \leq k-1\} \cup \{y_i \mid j+1 \leq i \leq n\}$. *Then* $cut(A_4, V \setminus A_4) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ *and* $Ncut(A_4, V \setminus A_4) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil \left(\frac{1}{(n-1)\lfloor \frac{n}{2} \rfloor} + \frac{1}{(n-1)\lceil \frac{n}{2} \rceil + 6} \right) = \frac{\lceil \frac{n}{2} \rceil (n^2 - n + 6)}{(n-1)^2 \lceil \frac{n}{2} \rceil + 6(n-1)}$.
We can deduce this as,

$$= \begin{cases} \frac{n(n^2-n+6)}{(n-1)(n^2-n+12)} & n \text{ even}, \\ \frac{(n^2-n+6)(n+1)}{(n-1)(n^2+11)} & n \text{ odd}. \end{cases}$$

Comparing Case(i) with Case(iv) for even n we have, $Case(i) - Case(iv) = \frac{(n^2 - n + 6)(-n^3 + 9n - 12)}{2(n^2 - n + 2)(n-1)(n^2 - n + 12)} < 0$ *for* $n \geq 3$. *Similarly, for odd n,* $Case(i) - Case(iv) = \frac{(n^2 - n + 6)(-n^3 - n^2 + 9n - 15)}{2(n^2 - 2n + 2)(n-1)(n^2 + 11)} < 0$ *for* $n \geq 3$. *Hence Case(i) is the minimum.*
Considering all cases, Case(i) has the minimum cut size and also the minimum normalized cut. Therefore $Mcut(LP'_{n,2}) = \frac{n^2 - n + 6}{2(n^2 - n + 2)}$ *for* $n \geq 3$.
The Figure 10 shows $Mcut(LP'_{n,2})$ *for* $n = 4, 6$. ■

2.7 Double tree cross path

In this section, we consider double tree cross path. Double tree cross path is a graph constructed by taking the Cartesian product of double tree with path. We derive a formula for $Mcut(DT_n \square P_m)(n \geq 2, m \geq 2)$.



(a) $LP'_{4,2}$ (b) $LP'_{6,2}$

Figure 10: $Mcut(LP'_{n,2})$ for $n = 4, 6$.

Proposition 2.8
Let $DT_n (n \geq 2)$ be a double tree of size $2^{n+1} - 2$, where n denotes the depth of the tree. Then

$$Mcut(DT_n \square P_m) = \begin{cases} \frac{2m}{(2m-1)2^{n+1}-5m+2} & \text{for } 2 \leq m < 2^{n+1} - 2, \\ \frac{(2^{n+1}-2)((2m-1)2^{n+2}-10m+4)}{(2^{n+3}-10)^2 \lfloor \frac{m}{2} \rfloor \lceil \frac{m}{2} \rceil - (2^{n+1}-2)(2^{n+3}-10)m + (2^{n+1}-2)^2} & \text{for } m \geq 2^{n+1} - 2. \end{cases}$$

(Proof) The size of a tree is $|T_n| = 1 + 2 + \cdots + 2^n = 2^n - 1$ and the size of a double tree is $|DT_n| = 2|T_n| = 2^{n+1} - 2$. The volume of a tree is $vol(T_n) = 2^{n+1} - 4$ and the volume of a double tree is $vol(DT_n) = 2vol(T_n) + 2 = 2^{n+2} - 6$. $DT_n \subset (DT_n \square P_m)$. Let $Y = 2^{n+1} - 2$. Then

$$\begin{aligned} |DT_n| &= Y, \text{ and} \\ vol(DT_n \square P_m) &= vol(DT_n)m + |DT_n|(2m-2) \\ &= (2^{n+2} - 6)m + 2(2^n - 1)(2m - 2) \\ &= (2m-1)2^{n+2} - 10m + 4 \\ &= 2Y(2m-1) - 2m. \end{aligned}$$

Case(i) *Let $A_1 = \{(x(w), p(i)) \mid 1 \leq i \leq m, w \in \Sigma^{\leq n}\}$ and $V \setminus A_1 = \{(y(w), p(i)) \mid 1 \leq i \leq m, w \in \Sigma^{\leq n}\}$. Then $A_1 = (T_n \square P_m)$ and*

$$\begin{aligned} vol(A_1) &= (vol(T_n) + 1)m + |T_n|(2m-2) \\ &= (2m-1)2^{n+1} - 5m + 2 \\ &= Y(2m-1) - m, \\ vol(V \setminus A_1) &= (2m-1)2^{n+1} - 5m + 2 \\ &= Y(2m-1) - m, \\ cut(A_1, V \setminus A_1) &= m. \end{aligned}$$

Therefore $Ncut(A_1, V \setminus A_1) = \dfrac{2m}{Y(2m-1) - m}$.

Case(ii) *Let $A_2 = \{(x(w), p(i)) \mid 1 \leq i \leq \lfloor \frac{m}{2} \rfloor, w \in \Sigma^{\leq n}\} \cup \{y(w), p(i)) \mid 1 \leq i \leq \lfloor \frac{m}{2} \rfloor, w \in \Sigma^{\leq n}\}$ and $V \setminus A_2 = \{(x(w), p(i)) \mid 1 + \lfloor \frac{m}{2} \rfloor \leq i \leq m, w \in \Sigma^{\leq n}\} \cup \{(y(w), p(i)) \mid 1 + \lfloor \frac{m}{2} \rfloor \leq i \leq m, w \in \Sigma^{\leq n}\}$.*

Then

$$\begin{aligned}
vol(A_2) &= vol(DT_n)\lfloor\frac{m}{2}\rfloor + |DT_n|(2\lfloor\frac{m}{2}\rfloor - 1)\\
&= (2^{n+2}-6)\lfloor\frac{m}{2}\rfloor + 2(2^n-1)(2\lfloor\frac{m}{2}\rfloor - 1)\\
&= (2.2^{n+2}-10)\lfloor\frac{m}{2}\rfloor - 2^{n+1} + 2\\
&= (4Y-2)\lfloor\frac{m}{2}\rfloor - Y,\\
vol(V\setminus A_2) &= (2.2^{n+2}-10)\lceil\frac{m}{2}\rceil - 2^{n+1} + 2,\\
&= (4Y-2)\lceil\frac{m}{2}\rceil - Y.
\end{aligned}$$

Then $Ncut(A_2, V\setminus A_2)$ *can be written as*

$$\begin{aligned}
&= \frac{|DT_n|vol(DT_n\Box P_m)}{(4Y-2)^2\lfloor\frac{m}{2}\rfloor\lceil\frac{m}{2}\rceil - (4Y-2)Ym + Y^2}\\
&= \frac{Y(4mY-2m-2Y)}{(4Y-2)^2\lfloor\frac{m}{2}\rfloor\lceil\frac{m}{2}\rceil - Y(4Y-2)m + Y^2}.
\end{aligned}$$

Case(iii)*Let* $A_3 = \{(x(w),p(i)) \mid 1\le i\le \lfloor\frac{m}{2}\rfloor, w\in\Sigma^{\le n}\}\cup\{(y(w),p(i)) \mid 1\le i\le\lfloor\frac{m}{2}\rfloor, w\in\Sigma^{\le n}\}\cup\{(x(w),p(1+\lfloor\frac{m}{2}\rfloor)) \mid w\in\Sigma^{\le n}\}$ *and* $V\setminus A_3 = \{(x(w),p(i)) \mid \lfloor\frac{m}{2}\rfloor+2\le i\le m, w\in\Sigma^{\le n}\}\cup\{(y(w),p(i)) \mid \lfloor\frac{m}{2}\rfloor+2\le i\le m, w\in\Sigma^{\le n}\}\cup\{(x(w),p(1+\lfloor\frac{m}{2}\rfloor)) \mid w\in\Sigma^{\le n}\}$. *Then*

$$\begin{aligned}
vol(A_3) &= vol(DT_n)\lfloor\frac{m}{2}\rfloor + |DT_n|(2\lfloor\frac{m}{2}\rfloor - 1) + vol(T_n) + 2|T_n| + 1\\
&= (2^{n+3}-10)\lfloor\frac{m}{2}\rfloor + 2^{n+1} - 3,\\
&= (4Y-2)\lfloor\frac{m}{2}\rfloor + Y - 1, \text{ and}
\end{aligned}$$

$$\begin{aligned}
vol(V\setminus A_3) &= vol(DT_n)(\lceil\frac{m}{2}\rceil - 1) + vol(T_n)|DT_n|(2(\lceil\frac{m}{2}\rceil - 1) - 1) + 2|T_n| + 1\\
&= (2^{n+3}-10)\lceil\frac{m}{2}\rceil - 3.2^{n+1} + 7,\\
&= (4Y-2)\lceil\frac{m}{2}\rceil - (3Y-1).
\end{aligned}$$

Then

$$\begin{aligned}
Ncut(A_3, V\setminus A_3) &= \frac{(|DT_n|+1)vol(DT_n\Box P_m)}{(4Y-2)^2\lfloor\frac{m}{2}\rfloor\lceil\frac{m}{2}\rceil - (4Y-2)(3Y-1)\lfloor\frac{m}{2}\rfloor + (Y-1)(4Y-2)\lceil\frac{m}{2}\rceil - (Y-1)(3Y-1)}\\
&= \frac{2(Y+1)(2mY-m-Y)}{(4Y-2)^2\lfloor\frac{m}{2}\rfloor\lceil\frac{m}{2}\rceil - (4Y-2)(3Y-1)\lfloor\frac{m}{2}\rfloor + (Y-1)(4Y-2)\lceil\frac{m}{2}\rceil - (Y-1)(3Y-1)}.
\end{aligned}$$

Case(iv) *Let* $A_4 = \{(x(w), p(i)) \mid 1 \le i \le \lfloor \frac{m}{2} \rfloor, w \in \Sigma^{\le n}\}$ *and* $V \setminus A_4 = \{(y(w), p(i)) \mid 1 \le i \le \lfloor \frac{m}{2} \rfloor, w \in \Sigma^{\le n}\} \cup \{(x(w), p(j)) \mid 1 + \lfloor \frac{m}{2} \rfloor \le j \le m, w \in \Sigma^{\le n}\} \cup \{(y(w), p(j)) \mid 1 + \lfloor \frac{m}{2} \rfloor \le j \le m, w \in \Sigma^{\le n}\}$. *Then*

$$\begin{aligned}
vol(A_4) &= (1 + vol(T_n))\lfloor \frac{m}{2} \rfloor + |T_n|(2\lfloor \frac{m}{2} \rfloor - 1) \\
&= (2^{n+2} - 5)\lfloor \frac{m}{2} \rfloor - 2^n + 1, \\
&= (2Y - 1)\lfloor \frac{m}{2} \rfloor - \frac{Y}{2}, \text{ and} \\
vol(V \setminus A_4) &= vol(DT_n)\lceil \frac{m}{2} \rceil + |DT_n|(2\lceil \frac{m}{2} \rceil - 1) + vol(A_4) \\
&= (2^{n+2} - 5)(2m - \lfloor \frac{m}{2} \rfloor) - 3.2^n + 3, \\
&= (2Y - 1)(2m - \lfloor \frac{m}{2} \rfloor) - \frac{3Y}{2}.
\end{aligned}$$

$$\begin{aligned}
cut(A_4, V \setminus A_4) &= (|T_n| + 1 + \lfloor \frac{m}{2} \rfloor) \\
&= \frac{Y}{2} + 1 + \lfloor \frac{m}{2} \rfloor \text{ and} \\
Ncut(A_4, V \setminus A_4) &= \frac{\frac{Y}{2} + 1 + \lfloor \frac{m}{2} \rfloor}{(2Y-1)^2(2m - \lfloor \frac{m}{2} \rfloor)\lfloor \frac{m}{2} \rfloor - (2Y-1)\lfloor \frac{m}{2} \rfloor \frac{3Y}{2} - \frac{Y}{2}(2Y-1)(2m - \lfloor \frac{m}{2} \rfloor) + \frac{3Y^2}{4}}.
\end{aligned}$$

Now we can compare all cases considered above.
Case(ii) can be written as

$$\begin{cases} \frac{2Y(2Ym - m - Y)}{((2Y-1)m - (3Y-1))((2Y-1)m + (Y-1))} & m \text{ is odd}, \\ \frac{2Y}{-Y + 2Ym - m} & m \text{ is even}. \end{cases}$$

If m *is even then,* $Case(i)/Case(ii) = \frac{m}{Y}$ *and* $\frac{m}{Y} < 1$, *if* $m < Y$. *That is for all even* m, *if* $m < 2^{n+1} - 2$ *then Case(i) is the minimum. If* m *is odd then,* $Case(i)/Case(ii) = \frac{m(1 - 3Y + m(-1 + 2Y))(-1 + Y + m(-1 + 2Y))}{Y(m + Y - 2mY)^2}$. $Case(i)/Case(ii) < 1$, *if* $2 \le m < Y$. *That is for odd* m, *if* $m < 2^{n+1} - 2$ *then Case(i) is the minimum.*
Case(iii) can be written as

$$\begin{cases} \frac{2(Y+1)}{((2Y-1)m - Y)} & m \text{ is odd}, \\ \frac{2(Y+1)((2Y-1)m - Y)}{(Y - 1 + m(2Y-1))(-3(Y+1) + m(2Y-1))} & m \text{ is even}. \end{cases}$$

Now compare Case(i) with Case(iii). If m *is odd then,* $Case(i)/Case(iii) = \frac{m}{1+Y} < 1$, *if* $m < (1 + Y)$. *That is* $m < 2^{n+1} - 1$. *Similarly, for even* m, $Case(i)/Case(iii) = \frac{m(-1 + Y + m(-1 + 2Y))(-3(1 + Y) + m(-1 + 2Y))}{(1 + Y)(m + Y - 2mY)^2} < 1$, *if* $2 \le m < Y$. *That is Case(i) is the*

minimum for $m < 2^{n+1} - 2$.
Next compare Case(i) with Case(iv). Case(iv) can be written as

$$\begin{cases} \frac{4(2+m+Y)}{-3Y+m(-3+6Y)} & m \text{ is even,} \\ \frac{4(Y+1+m)(-Y+m(2Y-1))}{(m(2Y-1)-3Y+1)(-5Y+1+m(6Y-3))} & m \text{ is odd.} \end{cases}$$

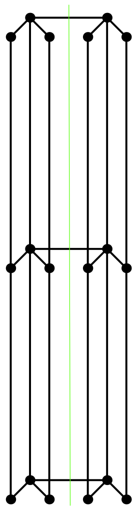
If m *is even then* $Case(i)/Case(iv) = \dfrac{3m}{2(2+m+Y)}$. $Case(i)/Case(iv) < 1$, *if* $m < 4 + 2Y$. *That is for* $m < 2^{n+2}$. *If* m *is odd then* $Case(i)/Case(iv) = \dfrac{m(1-3Y+m(-1+2Y))(1-5Y+m(-3+6Y))}{2(1+m+Y)(m+Y-2mY)^2}$. $Case(i)/Case(iv) < 1$ *if* $m < 2Y + 1$. *That is for* $m < 2^{n+1} + 3$, *Case(i) is the minimum.*

Claim 1 *If* $m < 2^{n+1} - 2$ *then, Case(i) is the minimum.*
Comparing Case(i) with Case(ii), $Case(i) < Case(ii)$ *for* $m < 2^{n+1} - 2$. *Comparing Case(i) with Case(iii),* $Case(i) < Case(iii)$, *for* $m < 2^{n+1} - 2$.
Comparing Case(i) with Case(iv), $Case(i) < Case(iv)$ *for* $m < 2^{n+2}$. *Hence the Case(i) is the minimum for* $m < 2^{n+1} - 2$.

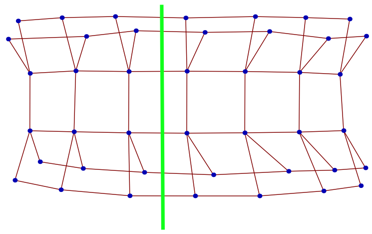
Next compare Case(ii) with Case(iii). If m *is odd then* $Case(ii)/Case(iii) = \dfrac{Y(m+Y-2mY)^2}{(1+Y)(1-3Y+m(-1+2Y))(-1+Y+m(-1+2Y))}$. $Case(ii)/Case(iii) < 1$, *if* $m \geq Y + 1$. *That is* $m \geq 2^{n+1} - 1$. *Since* m *is odd, Case(ii) is the minimum for odd* $m \geq 2^{n+1} - 2$. *If* m *is even then* $Case(ii)/Case(iii) = \dfrac{Y(-1+Y+m(-1+2Y))(-3(1+Y)+m(-1+2Y))}{(1+Y)(m+Y-2mY)^2}$. $Case(ii)/Case(iii) < 1$ *for* $m \geq 2$ *and* $Y \geq 1$. *That is for* $m \geq 2$ *and* $n \geq 2$. *Therefore Case(ii) is the minimum for* $m \geq 2^{n+1} - 2$. *Next we compare Case(ii) with Case(iv) for even m.* $Case(ii)/Case(iv) = \dfrac{3Y}{2(2+m+Y)}$. *That is* $Case(ii)/Case(iv) < 1$ *for* $m \geq 2^n - 3$. *If* m *is odd then* $Case(ii)/Case(iv) = \dfrac{Y(1-5Y+m(-3+6Y))}{2(1+m+Y)(-1+Y+m(-1+2Y))}$. $Case(ii)/Case(iv) < 1$ *for* $m \geq Y$. *That is for* $m \geq 2^{n+1} - 2$.

Claim 2 *If* $m \geq 2^{n+1} - 2$ *then Case(ii) is the minimum.*
Comparing Case(i) with Case(ii), Case(ii) is the minimum for $m \geq 2^{n+1} - 2$. *Comparing Case(ii) with Case(iii), Case(ii) gives minimum for* $m \geq 2^{n+1} - 2$ *Comparing Case(ii) with Case(iv), Case(ii) gives minimum for* $m \geq 2^n - 3$, *when* m *is even and* $m \geq 2^{n+1} - 2$ *when* m *is odd. Hence the Case(ii) is the minimum for* $m \geq 2^{n+1} - 2$.

Therefore Claim 1 and Claim 2 gives the required result. The Figure 11 shows Case(i) and Case(ii), where a green line indicates the bipartition. ∎



(a) $DT_2 \square P_3$



(b) $DT_2 \square P_7$

Figure 11: Double tree cross paths.

2.8 Conclusion

In this chapter, we discussed the properties of minimum normalized cut of some graph classes and derive a formula for $Mcut(G)$ *of graphs. Finding a formula for* $Mcut(G)$ *of graphs like* $R_{n,k}$,$P_{n,k}$,$LP_{n,m}$,$LP'_{n,2}$ *and double tree cross paths takes lot of time and the computation is also difficult.*

3 Difference Laplacian, normalized Laplacian, signless Laplacian and their eigenvalues

This chapter review the survey results of three Laplacian matrices called difference Laplacian, normalized Laplacian and signless Laplacian. Even most of these results are known, we try to summarize them by improving the readability. Specially we emphasize the second smallest eigenvalue of the normalized and difference Laplacian matrices and their boundary values using isoperimetric number, Cheeger constant, diameter etc. We give uniform proofs to find eigenvalues of paths and cycles of above three Laplacian matrices using circulant matrices and also give an alternate proof to find eigenvalues of an adjacency matrix of cycles and paths using Chebyshev polynomials. Our graphs are undirected but they may have loops and we assume that all graphs have edge weight one.

3.1 Difference Laplacian and bounds for the eigenvalues

In this section, we discuss the difference Laplacian matrix and the isoperimetric number $i(G)$ of a graph G. We show that the bounds for the second smallest eigenvalue λ_2 of difference Laplacian is,

$$\Delta - \sqrt{\Delta^2 - i(G)^2} \leq \lambda_2 \leq 2i(G).$$

Proposition 3.1
Let $L(G)$ be the difference Laplacian matrix of a weighted graph G and $f = (f_1, \ldots, f_n) \in \Re^n$ be an eigenvector. Then $\langle f, Lf \rangle$ can be written as

$$\langle f, Lf \rangle = \frac{\sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j)^2}{2}.$$

(Proof)

$$\begin{aligned}
f^T L f &= f^T (D - W) f \\
&= f^T D f - f^T W f \\
&= \sum_{i=1}^n f_i^2 d_i - \sum_{i=1}^n \sum_{j=1}^n f_i f_j w_{ij} \\
&= \frac{\left(\sum_{i=1}^n f_i^2 \sum_{j=1}^n w_{ij} + \sum_{j=1}^n f_j^2 \sum_{i=1}^n w_{ij}\right)}{2} - \sum_{i=1}^n \sum_{j=1}^n f_i f_j w_{ij} \\
&= \frac{\sum_{i=1}^n \sum_{j=1}^n \left(f_i^2 + f_j^2 - 2 f_i f_j\right) w_{ij}}{2} \\
&= \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2}.
\end{aligned}$$

■

Basic properties of difference Laplacian $L(G)$ are listed as follows.

- *$L(G)$ is a real symmetric matrix.*
- *$L(G)$ is positive semi-definite ($f^T L f \geq 0$).*

- $\lambda_i \geq 0, (i = 1, \dots, n)$.
- $\lambda_2(L(G)) = \min\{\langle Lf, f\rangle \; |f \in \Re^n, ||f|| = 1\}$.

Lemma 3.1
Let $G = (V, E)$ be a graph and $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of difference Laplacian matrix. Then $\lambda_2 > 0$ if and only if G is a connected graph.

(Proof) First assume that the graph is disconnected and has k connected components such that $G = \cup_{i=1}^{k} G_i$. Then we can write the difference Laplacian matrix as

$$L(G) = \begin{pmatrix} L(G_1) & 0 & \cdots & 0 \\ 0 & L(G_2) & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & \cdots & \cdots & L(G_k) \end{pmatrix}.$$

This is a block diagonal matrix and the characteristic polynomial of $P_{L(G)} = \prod_{i=1}^{k} P_{L(G_i)}$. For each connected component, zero is an eigenvalue. Since G has k connected components it has eigenvalue zero with multiplicity at least k and $\lambda_2 = 0$.
Now suppose that the graph is connected. Let $x = (x_1, \dots, x_n)$ be an eigenvector. Then

$$\lambda = \frac{\langle L(G)x, x\rangle}{\langle x, x\rangle} = \frac{x^T L(G)x}{x^T x}.$$

Then $x^T L(G)x = \dfrac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(x_i - x_j)^2}{2}$ implies that $x^T L(G)x = 0$, if $x_i = x_j$ for all pair of vertices i, j. Since the graph is connected $x_i = x_j$ implies that there exists a constant vector x. Hence the eigenvalue zero has an eigenvector $(1, \dots, 1)^T$. Hence all other eigenvalues are greater than zero and therefore $\lambda_2 > 0$. ■

The smallest non-zero eigenvalue of the difference Laplacian is called Fiedler value or algebraic connectivity. It tells how well a graph can be separated using the sign patterns of the second eigenvector. If λ_2 is too small then it is possible to cut the graph into 2 without cutting too many edges. If λ_2 is large then it needed to cut several edges. If λ_2 of a graph is large then the graph is called an expander graph.

Example 3.1
For a complete graph K_n with large n, eigenvalues of a difference Laplacian matrix are 0 and n with multiplicity $n-1$. We need to cut lot of edges in order to bipartition the graph. For a graph like path P_n, the second smallest eigenvalue of a difference Laplacian matrix is less than 1 and we need to cut only one edge to separate the graph.

Corollary 3.1
Let G be a graph, and $L(G)$ be its difference Laplacian. Then, the multiplicity of eigenvalue 0 is equal to the number of connected components of G.

■

Proposition 3.2
$L(K_n)$ has eigenvalue 0 with multiplicity 1 and n with multiplicity $n-1$.

(Proof) Let x be any vector orthogonal to the all ones vector. Consider the first row expansion of $L(K_n)x = \lambda x$.

$$\begin{aligned}\lambda x_1 &= (n-1)x_1 - \sum_{i=2}^{n} x_i \\ &= (n-1)x_1 - (\sum_{i=1}^{n} x_i - x_1) \\ \lambda &= n.\end{aligned}$$

Thus, x is an eigenvector with an eigenvalue n. ■

Lemma 3.2
Let $G = (V(G), E(G))$ and $H = (V(H), V(H))$ be graphs with difference Laplacian eigenvalues $\lambda_1, \ldots, \lambda_n$ and $\mu_1, \ldots, \mu_n$ and the eigenvectors $x_1, \ldots, x_n$ and $y_1, \ldots, y_m$ respectively. Then, for each $1 \leq i \leq n$, and $1 \leq j \leq m$, $G \Box H$ has an eigenvector z with an eigenvalue $\lambda_i + \mu_j$ such that $z(v,w) = x_i(v)y_j(w)$.

(Proof) Let L denote the difference Laplacian of $G \Box H$, d_v the degree of the node v in G, and d_w the degree of the node w in H. Consider a vertex (v,w) in the graph $G \Box H$. We test whether an eigenvector $z(v,w) = x_i(v)y_j(w)$ has an eigenvalue $\lambda_i + \mu_j$.

$$\begin{aligned}(Lz)(v,w) &= (d_v + d_w)(x_i(v)y_j(w)) - \sum_{(v,v_2)\in E(G)} (x_i(v_2)y_j(w)) - \sum_{(w,w_2)\in E(H)} (x_i(v)y_j(w_2)) \\ &= d_v(x_i(v)y_j(w)) - \sum_{(v,v_2)\in E(G)} (x_i(v_2)y_j(w)) + d_w(x_i(v)y_j(w)) - \sum_{(w,w_2)\in E(H)} (x_i(v)y_j(w_2)) \\ &= y_j(w)\left(d_v x_i(v) - \sum_{(v,v_2)\in E(G)} x_i(v_2)\right) + x_i(v)\left(d_w y_j(w) - \sum_{(w,w_2)\in E(H)} y_j(w_2)\right) \\ &= y_j(w)\lambda_i x_i(v) + x_i(v)\mu_j y_j(w) \\ &= (\lambda_i + \mu_j)x_i(v)y_j(w).\end{aligned}$$

Thus, the eigenvalues and the eigenvectors of the grid graph are completely determined by the eigenvalues and eigenvectors of the path graph. ■

Example 3.2 (The eigenvalues and the eigenvectors of the grid graphs)
Consider the grid graph shown in the Figure 12. Eigenvalues of difference Laplacian matrix of P_3 are $\{3,1,0\}$ and those of P_2 are $\{2,0\}$. Then the eigenvalues of $(P_3 \Box P_2)$ are $\{5,3,3,2,1,0\}$. Eigenvectors of difference Laplacian of P_3 are $\{(1,-2,1),(-1,0,1),(1,1,1)\}$ and P_2 are $\{(-1,1),(1,1)\}$. Then the eigenvectors of grid graph $(P_3 \Box P_2)$ are $\{(-1,2,-1,1,-2,1)$, $(1,-2,1,1,-2,1),(1,-2,1,1,-2,1),(-1,-1,-1,1,1,1),(-1,0,1,-1,0,1),(1,1,1,1,1,1)\}$.

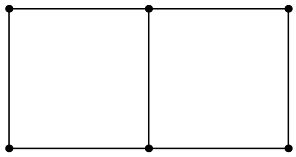


Figure 12: Grid graph $P_3 \Box P_2$.

Lemma 3.3
Let $G = (V(G), E(G))$ be a graph and $a, b \in V(G)$ be nonadjacent vertices. Then $\lambda_2(G) \leq \frac{1}{2}(d_a + d_b)$.

(Proof) Let $f \in \Re^{|V|}$ be defined by

$$f_i = \begin{cases} 1 & i = a, \\ -1 & i = b, \\ 0 & \textit{otherwise.} \end{cases}$$

Since

$$\begin{aligned} \lambda_2(G) &\leq \frac{\langle Lf, f\rangle}{\langle f, f\rangle} \\ &= \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2}{2\sum_i f_i^2} \\ &= \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i^2 + f_j^2 - 2f_i f_j)}{2(f_a^2 + f_b^2)} \\ &= \frac{\sum_{i=1}^{n} w_{i,a} f_a^2 + \sum_{j=1}^{n} w_{a,j} f_a^2 + \sum_{i=1}^{n} w_{i,b} f_b^2 + \sum_{j=1}^{n} w_{b,j} f_b^2}{4} \\ &= \frac{2(d_a + d_b)}{4} \\ &= \frac{d_a + d_b}{2}. \end{aligned}$$

■

Theorem 3.1
Let G be a graph with n vertices and f be an eigenvector of $L(G)$ with an eigenvalue $\lambda \neq 0$. Let G^c is a complement of G and its difference Laplacian is denoted by $L(G^c)$. Then f is an eigenvector of $L(G^c)$ with an eigenvalue $n - \lambda$.

(Proof) Let J be a $n \times n$ matrix with all entries equal to 1. $L(G) + L(G^c) = nI - J$ and $Jf = 0$ since $f \perp \vec{1}$. Then $nf = (nI - J)f = (L(G) + L(G^c))f = \lambda f + L(G^c)f$. Hence $L(G^c)f = (n - \lambda)f$. ■

Proposition 3.3
Isoperimetric numbers of the following graphs are discussed by Bojan Mohar 1989[34].

1. *The complete graph K_n, has $i(K_n) = \lceil \frac{n}{2} \rceil$.*

2. *The cycle C_n, has $i(C_n) = 2/\lfloor n/2 \rfloor$.*

3. *The path P_n, has $i(P_n) = 1/\lfloor n/2 \rfloor$.*

4. *The complete bipartite graph $K_{m,n}$ has its isoperimetric number equal to*

$$i(K_{m,n}) = \begin{cases} mn/(m+n) & \text{if } m \text{ and } n \text{ are even,} \\ (mn+1)/(m+n) & \text{if } m \text{ and } n \text{ are odd,} \\ mn/(m+n-1) & \text{if } m+n \text{ is odd,} \end{cases}$$

   which can be shortened to $i(K_{m,n}) = \dfrac{\lceil mn/2 \rceil}{\lfloor (m+n)/2 \rfloor}$.

5. *Petersen's graph has an isoperimetric number equal to 1.*

6. *The n-dimensional cube graph $Q_n = K_2^n$ has $i(Q_n) = 1$.*

Proposition 3.4
Let $G = (V(G), E(G))$ be a regular graph of degree r and $S \subseteq V(G)$. Then $r.h_G = i(G)$.

(Proof) By definition, $i(G) = \min_{S \subset V} \dfrac{cut(S, V \setminus S)}{\min(|S|, |V \setminus S|)}$ *and* $h_G = \min_{S \subset V} \dfrac{cut(S, V \setminus S)}{\min(vol(S), vol(V \setminus S))}$. *Then* $h_G = \min_{S \subset V} \dfrac{cut(S, V \setminus S)}{\min(r|S|, r|V \setminus S|)} = \dfrac{1}{r} i(G)$. *Hence we have $r.h_G = i(G)$.* ■

Proposition 3.5 (Mohar [35])
Let G be a weighted graph of order n. Then $\lambda_2(L(G)) = 2n \cdot \min\{\dfrac{\sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j)^2}{2\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2} \mid f \neq c\vec{1} \text{ for } c \in \Re\}$ *and* $\lambda_n(L(G)) = 2n \cdot \max\{\dfrac{\sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j)^2}{2\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2} \mid f \neq c\vec{1} \text{ for } c \in \Re\}$.

■

Lemma 3.4 (Mohar [35])
Let G be a weighted graph of order n and $S \subseteq V(G)$. Then $\lambda_2(G)\dfrac{|S|(n - |S|)}{n} \leq cut(S, V \setminus S) \leq \lambda_n(G)\dfrac{|S|(n - |S|)}{n}$.

(Proof) Let $f \in \Re^{|V|}$ be a function defined on $V(G)$ such that

$$f_i = \begin{cases} 1 & \text{if } i \in S, \\ 0 & \text{otherwise.} \end{cases}$$

Then $\sum_{i=1}^{n}\sum_{j=1}^{n}(f_i - f_j)^2 = \sum_{i\in S}\sum_{j\notin S}(f_i - f_j)^2 + \sum_{i\notin S}\sum_{j\in S}(f_i - f_j)^2 = 2|S|(n-|S|)$ *and*

$$\begin{aligned}
\frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2}{2} &= \frac{\sum_{i\in S, j\notin S} w_{ij}(f_i - 0)^2 + \sum_{i\notin S, j\in S} w_{ij}(0 - f_j)^2}{2} \\
&= \frac{\sum_{i\in S, j\notin S} w_{ij} + \sum_{i\notin S, j\in S} w_{ij}}{2} \\
&= cut(S, V\setminus S).
\end{aligned}$$

If $S \neq \emptyset$ *and* $S \neq V(G)$, *then* $\lambda_2(L(G)) \leq n \cdot \frac{cut(S,V\setminus S)}{|S|(n-|S|)}$ *by the Proposition 3.5. Similarly,* $\lambda_n(L(G)) \geq n \cdot \frac{cut(S,V\setminus S)}{|S|(n-|S|)}$ *by the Proposition 3.5. This shows the required result.* ■

Theorem 3.2 (Mohar [35])
Let G *be a graph on* n *vertices and let* λ_2 *be the second smallest eigenvalue of its difference Laplacian matrix. Then for every* k $(1 \leq k \leq n-1)$, $i_k(G) \geq \frac{(n-k)\lambda_2}{n}$ *and, consequently,* $i(G) \geq \frac{\lambda_2}{2}$.

(Proof) Let $X \subset V(G)$. *From the Lemma 3.4,*

$$\begin{aligned}
\lambda_2 &\leq cut(X, V\setminus X)\left(\frac{1}{|X|} + \frac{1}{|V\setminus X|}\right) \\
&= cut(X, V\setminus X)\left(\frac{n}{(n-k)k}\right)(k = |X|).
\end{aligned}$$

Since $i_k(G) \geq \frac{cut(X,V\setminus X)}{|X|}$, *we have* $i_k(G) \geq \frac{\lambda_2(n-k)}{n}$. *Further, if* $k \leq \frac{n}{2}$ *then* $\frac{(n-\frac{n}{2})}{n} \geq \frac{1}{2}$ *and we have* $i(G) \geq \frac{\lambda_2}{2}$. ■

Theorem 3.3 (Mohar [35])
Let $G = (V(G), E(G), w)$ *be a weighted graph of order* n, $G \neq K_n$, *and let* $\triangle = \triangle(G)$ *and* $\lambda_2 = \lambda_2(L(G))$. *Then* $i(G) \leq \sqrt{(2\triangle - \lambda_2)\lambda_2}$.

(Proof) Assume G *is a connected graph. Otherwise* $\lambda_2 = i(G) = 0$. *Let* $f = \{f_i \mid i \in V(G)\}$ *be an eigenvector of* λ_2 *such that* $S = \{i \in V(G) \mid f_i > 0\}$. *Assume that* $|S| \leq \frac{n}{2}$. *Let* $g = (g_1, \ldots, g_n) \in \Re^{|V|}$ *be defined by*

$$g_i = \begin{cases} f_i & \text{if } i \in S, \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$
\begin{aligned}
\lambda_2 \sum_{i\in S} f_i^2 &= \sum_{i\in S}(Lf)_i f_i \\
&= \sum_{i\in S}(d_i f_i - \sum_{j=1}^{n} w_{ij} f_j) f_i \ (L = D - W) \\
&= \sum_{i\in S}\sum_{j=1}^{n} w_{ij}(f_i - f_j) f_i \ (\textit{since } d_i = \sum_{j=1}^{n} w_{ij}) \\
&= \sum_{i\in S}\sum_{j\in S} w_{ij}(f_i - f_j) f_i + \sum_{i\in S}\sum_{j\notin S} w_{ij}\ (f_i - f_j) f_i \\
&\geq \sum_{i\in S}\sum_{j\in S} w_{ij}(f_i - f_j) f_i + \sum_{i\in S}\sum_{j\notin S} w_{ij} f_i^2 \ (f_i > 0 \textit{ and } f_j < 0) \\
&= \frac{\sum_{i\in S}\sum_{j\in S} w_{ij}((f_i - f_j) f_i + (f_j - f_i) f_j)}{2} + \sum_{i\in S}\sum_{j\notin S} w_{ij}(g_i - g_j)^2 \\
&= \frac{\sum_{i\in S}\sum_{j\in S} w_{ij}(g_i - g_j)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i - g_j)^2}{2} \\
&= \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i - g_j)^2}{2} = \langle Lg, g\rangle.
\end{aligned}
$$

Since $\sum_{i\in S} f_i^2 = \sum_{i=1}^{n} g_i^2 = \langle g, g\rangle$, *we have* $\lambda_2 \geq \frac{\langle Lg, g\rangle}{\langle g, g\rangle}$ *and let this as* K. *Then*

$$
\begin{aligned}
\frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i + g_j)^2}{2} &= \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i^2 + g_j^2) - \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w(i,j)(g_i - g_j)^2}{2} \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i^2 + g_j^2) - \langle Lg, g\rangle \\
&= 2\sum_{i=1}^{n} g_i^2 d_i - \langle Lg, g\rangle (\textit{substitute } d_i = \triangle) \\
&\leq 2\triangle \sum_{i=1}^{n} g_i^2 - \langle Lg, g\rangle \\
&= (2\triangle - K)\langle g, g\rangle.
\end{aligned}
$$

$$
\begin{aligned}
K &= \frac{\langle Lg, g\rangle}{\langle g, g\rangle} \\
&= \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i - g_j)^2 \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i + g_j)^2}{2\langle g, g\rangle \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(g_i + g_j)^2} \\
&\geq \frac{(\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}|g_i^2 - g_j^2|)^2}{4(2\triangle - K)\langle g, g\rangle^2} (\textit{numerator by Cauchy Schwarz}).
\end{aligned}
$$

Let us assign $M = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}|g_i^2 - g_j^2|$. *Let* $0 = t_0 < t_1 < \cdots < t_m$ *be all distinct values of* $g_i (i \in V(G))$. *For* $k = 0, 1, \ldots, m$, *let* $V_k := \{i \in V \mid g_i \geq t_k\}$. *Note that* $|V_k| \leq |S| \leq \frac{n}{2}$ *if* $k > 0$.

Then

$$\begin{aligned}
M &= \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}|g_i^2 - g_j^2| \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n}\{w_{ij}|g_i^2 - g_j^2 \mid g_i = t_k, j \notin V_k\} \\
&= 2\sum_{k=1}^{m}\sum_{i\in V_k}\sum_{j}\{w_{ij}(t_k^2 - t_{k-1}^2) \mid j \notin V_k\} \\
&= 2\sum_{k=1}^{m} cut(V_k, V \setminus V_k)(t_k^2 - t_{k-1}^2) \\
&\geq 2i(G)\sum_{k=1}^{m}|V_k|(t_k^2 - t_{k-1}^2) \\
&= 2i(G)\sum_{k=1}^{m} t_k^2(|V_k| - |V_{k+1}|)(Taking\ V_{m+1} = 0\ and\ by\ counting) \\
&= 2i(G)\sum_{i\in S} g_i^2.
\end{aligned}$$

Then we have, $K \geq \dfrac{i(G)^2}{2\triangle - K}$. *By expanding we have,* $K = \dfrac{-\triangle \pm\sqrt{4\triangle^2 - 4i(G)^2}}{-2} \geq 0$. $\lambda_2 \geq K$, *implies* $\lambda_2 \geq \triangle - \sqrt{\triangle^2 - i(G)^2}$. *Rearranging the terms, we have* $i(G)^2 \leq \lambda_2(2\triangle - \lambda_2)$. ∎

3.2 Normalized Laplacian

In this section, we analyze the basic properties of normalized Laplacian matrix and derive an upper bound and a lower bound for the second smallest eigenvalue of normalized Laplacian of a graph G, using Cheeger constant. The second smallest eigenvalue λ_2 *of normalized Laplacian of any graph G satisfies the following equation.*

$$1 - \sqrt{1 - h_G^2} \leq \lambda_2 \leq 2h_G.$$

3.2.1 Properties of normalized Laplacian

Lemma 3.5 ([10])
Let $G = (V, E, w)$ *be a weighted graph, where* $|V| = n$ and $W = (w_{ij})$ *be the weighted adjacency matrix. Let* $g = (g_1, \ldots, g_n) \in \Re^n$ *be an eigenvector and* $f = D^{-1/2}g$, *where* $D = D(G)$. *Then we have*

$$\frac{g^T\mathcal{L}g}{g^tg} = \frac{f^TLf}{f^TDf} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2}{2\sum_{i=1}^{n} f_i^2 d_i},$$

where $d_i = \sum_{j=1}^{n} w_{ij}$, $L = D - W$ and $\mathcal{L} = D^{-1/2} L D^{-1/2}$.

(Proof)

$$\frac{g^T \mathcal{L} g}{g^T g} = \frac{f^T D^{1/2} \mathcal{L} D^{1/2} f}{(D^{1/2} f)(D^{1/2} f)} = \frac{f^T L f}{f^T D f}.$$

$$\begin{aligned}
f^T L f &= f^T (D - W) f \\
&= f^T D f - f^T W f \\
&= \frac{\sum_{i=1}^{n} f_i^2 d_i - \sum_{i=1}^{n} \sum_{j=1}^{n} f_i f_j w_{ij}}{2} \\
&= \sum_{i=1}^{n} f_i^2 \sum_{j=1}^{n} w_{ij} - \sum_{i=1}^{n} \sum_{j=1}^{n} f_i f_j w_{ij} \\
&= \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} (f_i - f_j)^2 w_{ij}}{2} \\
f^T D f &= \sum_i f_i^2 d_i \\
\frac{f^T L f}{f^T D f} &= \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2}{2 \sum_{i=1}^{n} f_i^2 d_i}.
\end{aligned}$$

Note.

$$\begin{aligned}
\frac{\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2}{2} &= \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i^2 + f_j^2 - 2 f_i f_j)}{2} \\
&= \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i^2}{2} + \frac{\sum_{j=1}^{n} \sum_{i=1}^{n} w_{ij} f_j^2}{2} - \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i f_j \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} f_i^2 w_{ij} - f_i f_j w_{ij}.
\end{aligned}$$

■

If g is an eigenvector then $g \neq 0$ and $\mathcal{L}(G) g = \lambda g$. Hence $\langle g, \mathcal{L}(G) g \rangle = \langle g, \lambda g \rangle = \lambda \langle g, g \rangle$, and $\lambda = \dfrac{\langle g, \mathcal{L}(G) g \rangle}{\langle g, g \rangle}$. If λ is a zero eigenvalue then $\dfrac{f^T L f}{f^T D f} = 0$ implies that $\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2 = 0$. This happened when $f_i = f_j$ for all i, j. Hence the eigenvalue zero has a constant eigenvector which is $D^{1/2} \vec{1}$. The second eigenvector is orthogonal to the first eigenvector and we have $\langle D^{1/2} \vec{1}, g \rangle = \langle D^{1/2} \vec{1}, D^{1/2} f \rangle = D \langle 1, f \rangle = 0$. Hence the second smallest eigenvalue $\lambda_2 = \inf_{f \perp D \vec{1}} \dfrac{\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2}{2 \sum_{i=1}^{n} f_i^2 d_i}$.

Example 3.3

Let g be the second smallest eigenvector of $P_{2,3}$. Then $g = (-0.810313, -0.894013, -0.304918,$ $0.686214, 1)$. Then we can find $f = D^{-1/2} g$. Hence $\lambda_2 = \dfrac{f^T L f}{f^T D f} = 0.219854$.

Proposition 3.6
Let $g = (g_i)$ be an eigenvector of G such that $f = D^{-1/2}g$. Then the second smallest eigenvalue of the normalized Laplacian can be written as

$$\lambda_2 = \frac{\sum_{i=1}^n f_i \sum_{j=1}^n (f_i - f_j)w_{ij}}{\sum_{i=1}^n f_i^2 d_i}.$$

(Proof) We can write $(Lf)_i = \sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)w_{ij}$. *This follows from the fact that,* $(Lf)_i = ((D - W)f)_i = \sum_{i=1}^n d_i f_i - \sum_{i=1}^n \sum_{j=1}^n w_{ij} f_j = \sum_{i=1}^n f_i \sum_{j=1}^n w_{ij} - \sum_{i=1}^n \sum_{j=1}^n w_{ij} f_j = \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j)$. *By using this, we can write* λ_2 *as*

$$\begin{aligned}
\lambda_2 &= \inf_{g \perp D^{1/2}\vec{1}} \frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} \\
&= \inf_{f \perp D\vec{1}} \frac{f^T L f}{f^T D f} \\
&= \frac{\sum_{i=1}^n f_i (Lf)_i}{\sum_{i=1}^n f_i^2 d_i} \\
&= \frac{\sum_{i=1}^n f_i \sum_{j=1}^n (f_i - f_j)w_{ij}}{\sum_{i=1}^n f_i^2 d_i}.
\end{aligned}$$

■

Proposition 3.7
Let $g : V(G) \to \Re$. Then $(\mathcal{L}g)_i$ can be written as $(\mathcal{L}g)_i = \frac{1}{\sqrt{d_i}} \sum_{j=1}^n (\frac{g_i}{\sqrt{d_i}} - \frac{g_j}{\sqrt{d_j}})$.

(Proof)

$$\begin{aligned}
(\mathcal{L}g)_i &= g_i - \sum_{j=1, i \neq j}^n \frac{g_j}{\sqrt{d_i d_j}} \\
&= \sum_{j=1}^n (\frac{g_i}{d_i} - \frac{g_j}{\sqrt{d_i d_j}}) \\
&= \frac{1}{\sqrt{d_i}} \sum_{j=1}^n (\frac{g_i}{\sqrt{d_i}} - \frac{g_j}{\sqrt{d_j}})
\end{aligned}$$

■

Proposition 3.8
Let G be a k-regular graph G. Then $\mathcal{L}(G) = I - \frac{1}{k} \cdot A$.

(Proof) Let $\mathcal{L} = D^{-1/2}LD^{-1/2} = D^{-1/2}(D - A)D^{-1/2} = I - D^{-1/2}AD^{-1/2} = I - \frac{A}{k}$. ■

Lemma 3.6
For a graph G on n vertices we have,

(i) $\sum_{i=1}^{n} \lambda_i \leq n$ *with equality holds iff G has no isolated vertices.*

(ii) For $n \geq 2$, we have $\lambda_2 \leq \frac{n}{n-1}$ with equality holds iff G is a complete graph on n vertices. Also for a graph G without isolated vertices, we have $\lambda_{n-1} \geq \frac{n}{n-1}$.

(iii) For a graph G, which is not a complete graph, we have $\lambda_2 \leq 1$.

(iv) If G is connected then $\lambda_2 > 0$. If $\lambda_i = 0$ and $\lambda_{i+1} \neq 0$ then G has exactly i connected components.

(v) For all $i \leq n$, we have $\lambda_i \leq 2$ with $\lambda_n = 2$ iff a connected component of G is bipartite and nontrivial.

(Proof)

(i) If G is a connected graph without isolated vertices, we have $Trace(\mathcal{L}) = \sum_i \lambda_i = n$, where n is the total number of vertices. If there exists an isolated vertex then for each isolated vertex we have a zero row in the normalized Laplacian matrix. Hence $Trace(\mathcal{L}) < n$.

(ii) Consider above part (i) with $\lambda_1 = 0$. Then

$$\begin{aligned} \lambda_2 + \cdots + \lambda_n &= n \\ (n-1)\lambda_2 &\leq n, \end{aligned}$$

where λ_2 is the smallest non zero eigenvalue. Therefore $\lambda_2 \leq \frac{n}{n-1}$
Similarly,

$$\begin{aligned} \lambda_2 + \cdots + \lambda_n &\leq (n-1)\lambda_n \\ \lambda_n &\geq \frac{n}{n-1}, \end{aligned}$$

where λ_n is the largest eigenvalue.

(iii) Suppose G contains two non adjacent vertices a, b. Let

$$f_i = \begin{cases} d_b & i = a, \\ -d_a & i = b, \\ 0 & i \neq a, b. \end{cases}$$

$$\begin{aligned} \lambda_2 &= \inf_f \frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^{n} f_i^2 d_i} \\ &= \inf_f \frac{\sum_{j=1}^{n}(f_a - f_j)^2 w_{aj} + \sum_{j=1}^{n}(f_b - f_j)^2 w_{bj} + \sum_{i=1}^{n}(f_i - f_a)^2 w_{ia} + \sum_{i=1}^{n}(f_i - f_b)^2 w_{ib}}{2(f_a^2 d_a + f_b^2 d_b)} \\ &= \inf_f \frac{f_a^2 d_a + f_b^2 d_b}{f_a^2 d_a + f_b^2 d_b} \\ &= \inf_f 1. \end{aligned}$$

Hence $\lambda_2 \leq 1$.

(iv) *If G is connected then the eigenvalue 0 has multiplicity 1 since any eigenvector with the eigenvalue 0 assumes the same value at each vertex. Therefore $\lambda_2 > 0$. If G is a disconnected graph with i components then the eigenvalues of G are $\lambda(G) = \cup_i \lambda(G_i)$. For each connected graph, zero is an eigenvalue with multiplicity 1. If $\lambda_i = 0$ and $\lambda_{i+1} \neq 0$ then G has exactly i components.*

(v) *The largest eigenvalue λ_n satisfy the equation $\lambda_n = \sup_f \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2}{2\sum_i f_i^2 d_i}$. By using the fact that $(f_i - f_j)^2 \leq 2(f_i^2 + f_j^2)$, for all $1 \leq i \leq n$, we have $\lambda_i \leq \sup_f \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2}{2\sum_i f_i^2 d_i} \leq \frac{2\sum_{i=1}^n \sum_{j=1}^n (f_i^2 + f_j^2) w_{ij}}{2\sum_i f_i^2 d_i} = \frac{\sum_{i=1}^n f_i^2 d_i + \sum_{j=1}^n f_j^2 d_j}{\sum_i f_i^2 d_i} = \frac{2\sum_{i=1}^n f_i^2 d_i}{\sum_i f_i^2 d_i}$. Therefore $\lambda_i \leq 2$. Equality holds for $i = n$, when $f_i = -f_j (i = 1, \ldots, n)$ for every edge $(i, j) \in E(G)$. Since $f \neq 0$, G has a bipartite connected component. On the other hand if G has a bipartite connected component, we can choose the function f so as to make $\lambda_n = 2$.*

■

Lemma 3.7
The following statements are equivalent:

(i) *$G = (A, B, E)$ is a bipartite graph, where A, B are vertex sets and E is an edge set.*

(ii) *G has i connected components and $\lambda_{n-j} = 2$ for $0 \leq j \leq i - 1$.*

(iii) *For each λ_i the value $2 - \lambda_i$ is also an eigenvalue of G.*

(Proof)

1. *(i) → (ii). If G is a bipartite graph then $\lambda_n = 2$. If G is a disconnected graph with i bipartite connected components then $\lambda(G) = \cup_i \lambda(G_i)$. For each i, $\lambda_n(G_i) = 2$ from the Lemma 3.6-(v). That is $\lambda_{n-j} = 2$ for $0 \leq j \leq i - 1$.*

2. *(i) → (iii). Let G is a bipartite graph with a vertex set A and B such that $m = |A|$ and $n = |B|$. Let $g = D^{-1/2} f$. Then define g as*

$$g_i = \begin{cases} f_i & \text{if } i \in A, \\ -f_i & \text{if } i \in B. \end{cases}$$

Then

$$\lambda_2 = \inf_f \frac{\sum_{i=1}^{m+n} \sum_{j=1}^{m+n} (f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^{m+n} f_i^2 d_i}.$$

Let λ_f be an eigenvalue. Then

$$\begin{aligned}
\lambda_f &= \frac{\sum_{i=1}^{m+n}\sum_{j=1}^{m+n}(f_i-f_j)^2 w_{ij}}{2\sum_{i=1}^{m+n} f_i^2 d_i} \\
\lambda_f &= \frac{\sum_{i=1}^{m+n} f_i^2 \sum_{j=1}^{m+n} w_{ij} + \sum_{j=1}^{m+n} f_j^2 \sum_{i=1}^{m+n} w_{ij} - 2\sum_{i=1}^{m+n}\sum_{j=1}^{m+n} f_i f_j w_{ij}}{2(\sum_{i=1}^{m+n} f_i^2 d_i + \sum_{j=1}^{m+n} f_j^2 d_j)} \\
\lambda_f &= \frac{2\sum_{i=1}^{n+m} f_i^2 d_i - 2\sum_{i=1}^{m+n}\sum_{j=1}^{m+n} f_i f_j w_{ij}}{2\sum_{i=1}^{n+m} f_i^2 d_i} \\
&= 1 - \frac{\sum_{i=1}^{n}\sum_{j=1}^{m+n} f_i f_j w_{ij}}{\sum_{i=1}^{n+m} f_i^2 d_i}.
\end{aligned}$$

If g is an eigenvector then

$$\begin{aligned}
\lambda_g &= 1 - \frac{\sum_{i=1}^{m+n}\sum_{j=1}^{m+n} g_i g_j w_{ij}}{\sum_{i=1}^{n+m} g_i^2 d_i} \\
\lambda_g &= 1 + \frac{\sum_{i=1}^{m+n}\sum_{j=1}^{m+n} f_i f_j w_{ij}}{\sum_{i=1}^{n+m} f_i^2 d_i} \\
\lambda_g &= 2 - \lambda_f.
\end{aligned}$$

Whenever λ_f is an eigenvalue then $2-\lambda_f$ is also an eigenvalue.

■

3.2.2 Cheeger constant of graphs

Proposition 3.9 (Fan Chung [10])
Let G be a connected graph. Then $h_G > \dfrac{2}{vol(G)}$.

■

Lemma 3.8 (Fan Chung[10])
Let G be a connected graph with diameter $diam(G)$. Then we have $\lambda_2 \geq \dfrac{1}{diam(G)vol(G)}$.

(Proof) Let $g = (g_1, g_2, \ldots, g_n)$ be the second eigenvector such that $g = D^{1/2}f$. Let $f_{i_0} = \max_i |f_i|$. Then $\lambda_2 = \dfrac{\sum_{i=1}^{n}\sum_{j=1}^{n}(f_i-f_j)^2 w_{ij}}{2\sum_i f_i^2 d_i}$. Since the second eigenvector is orthogonal to $D^{1/2}\vec{1}$, $\displaystyle\sum_i f_i d_i = \sum_i \frac{g_i}{\sqrt{d_i}} d_i = 0$ and there exists a vertex j_0 such that $f_{i_0} f_{j_0} < 0$. Let P denote the shortest path from

i_0 to j_0. Then $\sum_i f_i^2 d_i \le f_{i_0}^2 \sum_i d_i = f_{i_0}^2 vol(G)$.

$$
\begin{aligned}
\lambda_2 &= \inf_{f \perp D\vec{1}} \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2\sum_i f_i^2 d_i} \\
&\ge \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2f_{i_0}^2 vol(G)} \\
&\ge \frac{2\sum_{(i,j)\in P} (f_i - f_j)^2 w_{ij}}{2f_{i_0}^2 vol(G)} \\
\text{By Cauchy Schwarz inequality} & \\
(\sum_{(i,j)\in P} (f_i - f_j) w_{ij})^2 &\le \sum_{(i,j)\in P} 1 \sum_{(i,j)\in P} (f_i - f_j)^2 w_{ij} \\
&= diam(G) \sum_{(i,j)\in P} (f_i - f_j)^2 w_{ij} \\
&\ge \frac{\frac{1}{diam(G)} (f_{i_0} - f_{j_0})^2}{vol(G) f_{i_0}^2} \quad (f_{i_0} f_{j_0} < 0) \\
&\ge \frac{1}{diam(G) vol(G)}.
\end{aligned}
$$

■

Lemma 3.9 (Fan Chung 1997 [10])
Let G be a connected graph. Then we have $\frac{h_G^2}{2} < \lambda_2 \le 2h_G$.

(Proof) (Right hand side) Let A and $V \setminus A$ be two partitions of G such that Cheeger constant h_G is optimal. Let $C = \{(v_i, v_j) \in E(G) \mid i \in A, j \in V \setminus A\}$. Let $g = (g_1, g_2, \ldots, g_n) \in \Re^n$ be an eigenvector and $f = D^{-1/2} g$.
Define f as ,

$$
f_i = \begin{cases} \frac{1}{vol(A)} & \text{if } i \text{ is in } A, \\ -\frac{1}{vol(V\setminus A)} & \text{if } i \text{ is in } V \setminus A. \end{cases}
$$

By substituting f in $\lambda_2 = \inf_{f \perp D\vec{1}} \frac{\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j)^2 w_{ij}}{2\sum_{i=1}^n f_i^2 d_i}$ *we have,*

$$
\begin{aligned}
\lambda_2 &\le \frac{2(\frac{1}{vol(A)} + \frac{1}{vol(V\setminus A)})^2 \sum_{i\in A, j \in V\setminus A} w_{ij}}{2((\frac{1}{vol(A)})^2 vol(A) + (\frac{1}{vol(V\setminus A)})^2 vol(V \setminus A))} \\
&\le |C| \left(\frac{1}{vol(A)} + \frac{1}{vol(V \setminus A)} \right) \\
&\le \frac{2|C|}{\min(vol(A), vol(V \setminus A))} \\
&= 2h_G.
\end{aligned}
$$

$\blacksquare$

Next we prove the left hand side of the equation.
(Left hand side) Relabel the vertices such that $f_i \leq f_{i+1}$ *for* $1 \leq i \leq n-1$. *Assume that*

$$\sum_{f_i<0} d_i \geq \sum_{f_j \geq 0} d_j$$

For each i, $1 \leq i \leq |V|$, *consider the cut*

$$C_i = \{(v_j, v_k) \in E(G) \mid 1 \leq j \leq i < k \leq n\}.$$

Define α *by*

$$\alpha = \min_{1 \leq i \leq n} \frac{|C_i|}{\min(\sum_{j \leq i} d_j, \sum_{j>i} d_j)}$$

Then it is clear that $\alpha \geq h_G$
Define the set of vertices V_+ *and* V_- *such that* $V_+ = \{i \in V(G) \mid f_i \geq 0\}$, $V_- = \{i \in V(G) \mid f_i < 0\}$ *and the set of edges* E_+, E_- *such that* $E_+ = \{(i,j) \in E(G) \mid i \in V_+ \text{ or } j \in V_+\}$ *and* $E_- = \{(i,j) \in E(G) \mid i \in V_- \text{ or } j \in V_-\}$.

Define g *as*

$$g_i = \begin{cases} f_i & i \in V_+, \\ 0 & \text{otherwise.} \end{cases}$$

By definition,

$$\lambda_2 = \inf_{f \perp D\vec{1}} \frac{\sum_{i=1}^n f_i \sum_{j=1}^n (f_i - f_j)}{\sum_{i=1}^n f_i^2 d_i}$$

By using vertex arrangement we can write this as,

$$\lambda_2 = \frac{\sum_{i \in V_+} f_i \sum_{(i,j) \in E_+} (f_i - f_j) + \sum_{i \in V_-} f_i \sum_{(i,j) \in E_-} (f_i - f_j)}{\sum_{i \in V_+} f_i^2 d_i + \sum_{i \in V_-} f_i^2 d_i}$$

Since $\dfrac{a+b}{c+d} \geq \min\{\dfrac{a}{c}, \dfrac{b}{d}\}$ *for* $a,b,c,d \in \Re$, *we have,*

$$\lambda_2 \geq \min\{\frac{\sum_{i \in V_+} f_i \sum_{(i,j) \in E_+} (f_i - f_j)}{\sum_{i \in V_+} f_i^2 d_i}, \frac{\sum_{i \in V_-} f_i \sum_{(i,j) \in E_-} (f_i - f_j)}{\sum_{i \in V_-} f_i^2 d_i}\}$$

Lets write this as $\lambda_2 \geq \min\{\lambda_2^+, \lambda_2^-\}$ *Assume that* $\lambda_2^+ \leq \lambda_2^-$. *Then we have*

$$\lambda_2 \geq \frac{\sum_{i \in V_+} f_i \sum_{(i,j) \in E_+} (f_i - f_j)}{\sum_{i \in V_+} f_i^2 d_i}.$$

Now we have,

$$\begin{aligned}
\lambda_2 &\geq \frac{\sum_{i\in V_+} f_i \sum_{(i,j)\in E_+}(f_i - f_j)}{\sum_{i\in V_+} f_i^2 d_i} \\
&= \frac{\sum_{(i,j)\in E_+}(g_i - g_j)^2}{\sum_{i\in V_+} g_i^2 d_i} \\
&= \frac{\sum_{(i,j)\in E_+}(g_i - g_j)^2 \sum_{(i,j)\in E_+}(g_i + g_j)^2}{\sum_{i\in V_+} g_i^2 d_i \sum_{(i,j)\in E_+}(g_i + g_j)^2} \\
&\quad (\mathit{Multiply\ the\ denominator\ and\ the\ numerator\ by} \sum_{(i,j)\in E_+}(g_i + g_j)^2) \\
&\geq \frac{(\sum_{(i,j)\in E_+}(g_i - g_j)(g_i + g_j))^2}{\sum_{i\in V_+} g_i^2 d_i \sum_{(i,j)\in E_+}(g_i + g_j)^2} \ (\mathit{By\ Cauchy\ Schwarz}) \\
&\geq \frac{(\sum_{(i,j)\in E_+}(g_i - g_j)(g_i + g_j))^2}{2(\sum_{i\in V_+} g_i^2 d_i)^2} \\
&= \frac{(\sum_{(i,j)\in E_+}|g_i^2 - g_j^2|)^2}{2(\sum_{i\in V_+} g_i^2 d_i)^2} \\
&\geq \frac{(\sum_{i=1}^n |g_i^2 - g_{i+1}^2||C_i|)^2}{2(\sum_{i\in V_+} g_i^2 d_i)^2} \\
&\geq \frac{(\sum_{i=1}^n |g_i^2 - g_{i+1}^2|\alpha \sum_{j\leq i} d_j)^2}{2(\sum_{i\in V_+} g_i^2 d_i)^2} \\
&\geq \frac{\alpha^2}{2} \\
&\geq \frac{h_G^2}{2}.
\end{aligned}$$

Further by using the Theorem 3.4, $\lambda_2 > 1 - \sqrt{1 - h_G^2} > \frac{h_G^2}{2}$ *and thus the* $\lambda_2 > \frac{h_G^2}{2}$ *holds. Note that*

$$\begin{aligned}
\sum_{i\in V^+} g_i^2 d_i (\sum_{(i,j)\in E_+}(g_i + g_j)^2) &= \sum_{i\in V^+} g_i^2 d_i (\sum_{(i,j)\in E_+} 2(g_i^2 + g_j^2) - (g_i - g_j))^2) \\
&= \sum_{i\in V^+} g_i^2 d_i (\sum_{(i,j)\in E_+} 2(g_i^2 d_i) - (g_i - g_j)^2) \\
&= 2(\sum_{i\in V^+} g_i^2 d_i)^2 - \sum_{i\in V^+} g_i^2 d_i \sum_{(i,j)\in E_+}(g_i - g_j)^2 \\
&\leq 2(\sum_{i\in V^+} g_i^2 d_i)^2.
\end{aligned}$$

■

Theorem 3.4
Let G be a connected graph. Then we have $\lambda_2 > 1 - \sqrt{1 - h_G^2}$.

From the proof of Lemma 3.9 we have, $\lambda_2 \geq \frac{\sum_{(i,j)\in E_+}(g_i-g_j)^2}{\sum_{i\in V_+} g_i^2 d_i} = W$. *Then we have,* $\sum_{(i,j)\in E_+}(g_i - g_j)^2 = W\sum_{i\in V_+} g_i^2 d_i$ *and* $\sum_{(i,j)\in E_+}(g_i+g_j)^2 = \sum_{(i,j)\in E_+} 2(g_i^2+g_j^2) - (g_i-g_j)^2 = \sum_{i\in V_+} 2g_i^2 d_i - \sum_{(i,j)\in E_+}(g_i - g_j)^2 = 2\sum_{i\in V_+} g_i^2 d_i - W\sum_{i\in V_+} g_i^2 d_i$. *Now we have,*

$$\begin{aligned} W &= \frac{\sum_{(i,j)\in E_+}(g_i-g_j)^2 \sum_{(i,j)\in E_+}(g_i+g_j)^2}{\sum_{i\in V_+} g_i^2 d_i \sum_{(i,j)\in E_+}(g_i+g_j)^2} \\ &\geq \frac{(\sum_{(i,j)\in E_+}|g_i^2-g_j^2|)^2}{(\sum_{i\in V_+} g_i^2 d_i)(2\sum_{i\in V_+} g_i^2 d_i - W\sum_{i\in V_+} g_i^2 d_i)} \; (Cauchy\ Schwarz) \\ &\geq \frac{(\sum_{i\in V_+}|g_i^2-g_{i+1}^2||C_i|)^2}{(2-W)(\sum_i g_i^2 d_i)^2} \\ &\geq \frac{\alpha^2}{(2-W)} \frac{(\sum_{i\in V_+}|g_i^2-g_{i+1}^2|\sum_{j\leq i} d_j)^2}{(\sum_i g_i^2 d_i)^2} \\ &\geq \frac{\alpha^2}{(2-W)}. \end{aligned}$$

This implies that $W^2 - 2W + \alpha^2 \leq 0$ *and we have* $\lambda_2 \geq W \geq 1 - \sqrt{1-h_G^2}$. ■

Proposition 3.10 (Fan Chung[10])
For a connected graph G, $\lambda_2 > \frac{g_G^2}{4\triangle + 2\triangle g_G}$, *where* $\triangle$ *is the maximum degree.*

■

Proposition 3.11 (Fan Chung [10])
Let G be a graph with diameter $diam(G) \geq 4$ *and* $\triangle$ *be the maximum degree. Then* $\lambda_2 \leq 1 - 2\frac{\sqrt{\triangle-1}}{\triangle}\left(1 - \frac{2}{diam(G)}\right) + \frac{2}{diam(G)}$.

■

3.2.3 Bounds for the normalized eigenvalues of paths

Proposition 3.12
Cheeger constant of a path P_n *is* $\frac{1}{2\lfloor\frac{n}{2}\rfloor - 1}$. *This can be written as*

$$h_{P_n} = \begin{cases} \frac{1}{n-1} & n \text{ even}, \\ \frac{1}{n-2} & n \text{ odd}. \end{cases}$$

(Proof) Consider the set A and $V \setminus A$ with the number of edges between them equal to 1. Suppose $|A| \leq |V \setminus A|$. In this case $|V \setminus A| \geq \lceil \frac{n}{2} \rceil$ and

$$\begin{aligned} h_G &= \min \frac{cut(A, V \setminus A)}{\min(vol(A), vol(V \setminus A))} \\ &= \frac{1}{\min(2\lfloor \frac{n}{2} \rfloor - 1, 2\lceil \frac{n}{2} \rceil - 1)} \\ &= \frac{1}{2\lfloor \frac{n}{2} \rfloor - 1}. \end{aligned}$$

Further we can write this as

$$h_{P_n} = \begin{cases} \frac{1}{n-1} & n \text{ even}, \\ \frac{1}{n-2} & n \text{ odd}. \end{cases}$$

■

Proposition 3.13
Vertex expansion of Cheeger constant of a path P_n is $\dfrac{2}{2\lfloor \frac{n}{2} \rfloor - 1}$. This can be written as

$$g_{P_n} = \begin{cases} \frac{2}{n-1} & n \text{ even}, \\ \frac{2}{n-2} & n \text{ odd}. \end{cases}$$

■

Corollary 3.2
Second smallest eigen value λ_2 of $\mathcal{L}(P_{4k})$ is $1 - \cos(\dfrac{\pi}{4k-1}) \approx \dfrac{\pi^2}{2(4k-1)^2}$(small angle approximation). Then we have $\dfrac{1}{2(4k-1)^2} \leq \lambda_2 \leq \dfrac{2}{4k-1}$ by Lemma 3.9.

■

Corollary 3.3
For a path graph P_{4k}, $\lambda_2 > \dfrac{4}{(4k-1)^2(4*2+2*2*\frac{2}{4k-1})} = \dfrac{1}{8k(4k-1)}$ by the Proposition 3.10.

■

Corollary 3.4
For a path graph P_{4k}, $\lambda_2 \leq \dfrac{4}{4k-1}$ by the Proposition 3.11.

■

Corollary 3.5
For a path graph P_{4k}, $\lambda_2 \geq \dfrac{1}{(4k-1)(8k-2)}$ by the Lemma 3.8.

■

3.2.4 Bounds for the normalized eigenvalues of weighted paths

Proposition 3.14
Cheeger constant of a weighted path $G = P_{2k,k}$ is given by $h_{P_{2k,k}} \geq \dfrac{2}{7k-2}$.

(Proof) **Case(i)** *Let $A \subseteq V(P_{2k,k})$ such that $A = \{x_i \mid 1 \leq i \leq 2k\}$ and $V \setminus A = \{x_i \mid 2k+1 \leq i \leq 3k\}$.* $h_G(A) = \dfrac{1}{\min(4k-1, 3k-1)} = \dfrac{1}{3k-1}$.
Case(ii) *Let $A_1 = \{x_i \mid 1 \leq i \leq \alpha\}$, where $2k < \alpha < 3k$ and $V \setminus A_1 = \{x_i \mid \alpha+1 \leq i \leq 3k\}$.* $h_G(A_1) = \dfrac{1}{\min(4k-2+3(\alpha-2k), 3(3k-\alpha)-1)} = \dfrac{1}{9k-1-3\alpha}$, $(2k < \alpha < 3k)$. *Now compare the Case(i) with Case(ii).* $(3k-1) - (9k-1-3\alpha) > 0$ *and the Case(i) is minimum among two.*
Case(iii) *Consider the set such that $A_2 = \{x_i \mid 1 \leq i \leq \alpha\}$, where $1 \leq \alpha < 2k$ and $V \setminus A_2 = \{x_i \mid \alpha + 1 \leq i \leq 3k\}$.* $h_G(A_2) = \dfrac{1}{\min(2\alpha-1, 3k-1+2(2k-\alpha))}$. *Then we have* $2\alpha - 1 - (3k-1+4k-2\alpha) = 4\alpha - 7k$. *If* $k \leq \dfrac{4\alpha}{7}$ *then* $h_G(A_2) = \dfrac{1}{7k-1-2\alpha}$.

$$\min\{2\alpha-1, 7k-1-2\alpha\} = \begin{cases} \frac{1}{7k-1-2\alpha} & k \leq \frac{4\alpha}{7}, \\ \frac{1}{2\alpha-1} & k \geq \frac{4\alpha}{7}. \end{cases}$$

For $k \leq \dfrac{4\alpha}{7}$, *we have a minimum at* $\dfrac{2}{7k-2}$. *For* $k \geq \dfrac{4\alpha}{7}$, *we have a minimum at* $\dfrac{2}{7k-2}$. *Comparing this value with* $\dfrac{1}{3k-1}$ *in the Case(i),* $\min\{\dfrac{1}{3k-1}, \dfrac{2}{7k-2}\} = \dfrac{2}{7k-2}$. *Then* $h_{P_{2k,k}} \geq \dfrac{2}{7k-2}$. ■

Corollary 3.6
For a connected graph $P_{2k,k}$, we have $\dfrac{1}{2(7k-2)^2} \leq \lambda_2 < \dfrac{4}{(7k-2)}$.

■

Corollary 3.7
For a connected graph $P_{2k,k}$ with diameter $diam(P_{2k,k}) = (3k-1)$, we have $\lambda_2 \geq \dfrac{1}{(3k-1)(7k-2)}$.

■

Corollary 3.8
For a connected graph $P_{2k,k}$ with diameter $diam(P_{2k,k}) = (3k-1)$, we have $\lambda_2 \leq 1 - \dfrac{2}{3k-1}\left(\sqrt{2}(k-1)-1\right)$.

■

3.2.5 Bounds for the normalized eigenvalues of $R_{2k,k}$

Proposition 3.15 (Cheeger constant of $R_{2k,k}$)
The Cheeger constant of $R_{2k,k}$ is $\dfrac{1}{4k-1}$.
(Proof) **Case(i)** $A_1 = \{x_i \mid 1 \leq i \leq 2k\}$ *and* $V \setminus A_1 = \{y_i \mid 1 \leq i \leq 3k\} \cup \{x_i \mid 2k+1 \leq i \leq 3k\}$.

$h_G(A_1) = \dfrac{1}{\min(4k-1, 10k-3)} = \dfrac{1}{4k-1}$.

Case(ii) $A_2 = \{x_i \mid 1 \le i \le 2k+\alpha\} \cup \{y_i \mid 1 \le i \le 2k+\alpha\}$, *where* $0 \le \alpha < k$ *and* $V \setminus A_2 = \{x_i \mid 2k+\alpha+1 \le i \le 3k\} \cup \{y_i \mid 2k+\alpha+1 \le i \le 3k\}$. $h_G(A_2) = \dfrac{2}{\min(8k-2+6\alpha, 6k-6\alpha-2)} = \dfrac{2}{6k-6\alpha-2}$. *considering Case(i), Case(ii),* $h_G = \min\{\dfrac{1}{4k-1}, \dfrac{1}{3k-3\alpha-1}\} = \dfrac{1}{4k-1}$, *since* $\dfrac{1}{4k-1} - \dfrac{1}{3k-3\alpha-1} = \dfrac{-(k+3\alpha)}{(4k-1)(3(k-\alpha)-1} < 0$.

Case(iii) $A_3 = \{x_i \mid 1 \le i \le 2k\} \cup \{y_i \mid 1 \le i \le 2k\}$ *and* $V \setminus A_3 = \{x_i \mid 2k+1 \le i \le 3k\} \cup \{y_i \mid 2k+1 \le i \le 3k\}$. $h_G(A_3) = \dfrac{2}{\min(2(4k-1), 2(3k-1))} = \dfrac{2}{6k-2}$. *Comparing Case(iii) with Case(i), Case(i) is the minimum.*

Case(iv) *Let* $A_4 = \{x_i \mid 1 \le i \le 3k\}$ *and* $V \setminus A_4 = \{y_i \mid 1 \le i \le 3k\}$. *Then* $vol(A_4) = vol(V \setminus A_4) = 7k-2$ *and* $h_G(A_4) = \dfrac{k}{7k-2}$. *Comparing with Case(i), Case(i) is the minimum.*

Case(v) *Let* $A_5 = \{x_i \mid 1 \le i \le \alpha\} \cup \{y_i \mid 1 \le i \le \alpha\}$, *where* $1 \le \alpha < 2k$ *and* $V \setminus A_5 = \{x_i \mid \alpha+1 \le i \le 3k\} \cup \{y_i \mid \alpha+1 \le i \le 3k\}$. $h_G(A_5) = \dfrac{2}{\min(4\alpha-2, 14k-4\alpha-2)}$

$$\min(4\alpha-2, 14k-4\alpha-2) = \begin{cases} 14k-4\alpha-2 & \frac{7k}{4} \le \alpha \le 2k, \\ 4\alpha-2 & \text{otherwise.} \end{cases}$$

and

$$h_G(A_5) = \begin{cases} \frac{2}{14k-4\alpha-2} & \frac{7k}{4} \le \alpha \le 2k, \\ \frac{2}{4\alpha-2} & \text{otherwise.} \end{cases}$$

Now compare Case(v) with Case(i).

$\min(\dfrac{1}{2\alpha-1}, \dfrac{1}{4k-1}) = \dfrac{1}{4k-1}$ *and* $\min(\dfrac{1}{7k-2\alpha-1}, \dfrac{1}{4k-1}) = \dfrac{1}{4k-1}$ *implies that the Case(i) is the minimum. Considering all cases above, Cheeger constant of* $R_{2k,k}$ *is* $\dfrac{1}{4k-1}$.

■

Corollary 3.9
For the graph $R_{2k,k}$, $\dfrac{1}{2(4k-1)^2} \le \lambda_2(\mathcal{L}(R_{2k,k})) \le \dfrac{2}{4k-1}$.

■

Corollary 3.10
For the graph $R_{2k,k}$, $\lambda_2(\mathcal{L}(R_{2k,k})) \ge \dfrac{1}{diam(R_{2k,k})vol(R_{2k,k})} = \dfrac{1}{2(4k+1)(7k-2)}$.

■

Corollary 3.11
For the graph $R_{2k,k}$, $\lambda_2(\mathcal{L}(R_{2k,k})) > 1 - \sqrt{1 - \dfrac{1}{(4k-1)^2}} = 1 - \dfrac{2\sqrt{(4k-2)k}}{4k-1}$ *by the Theorem 3.4.*

■

Corollary 3.12
For the graph $R_{2k,k}$, $\lambda_2(\mathcal{L}(R_{2k,k})) \leq 1 - 2\frac{\sqrt{3}-1}{3}\left(1 - \frac{2}{4k+1}\right) + \frac{2}{4k+1} = 1 - \frac{2}{4k+1}\left(\frac{4\sqrt{2}k - \sqrt{2} - 3}{3}\right)$.

■

Lemma 3.10 ([24])
Let A be a real symmetric matrix and A_r denote any $r \times r$ principal sub matrix of A. For any integer k such that $1 \leq k \leq r$, we have $\lambda_k(A) \leq \lambda_k(A_r) \leq \lambda_{k+n-r}(A)$.

Corollary 3.13
Let $R_{n,k}$ be a graph with $n + k$ vertices. Then $\lambda_2(\mathcal{L}(R_{n-1,k+1})) < \lambda_2(\mathcal{L}(R_{n,k}))$ for $n < k$ and $\lambda_2(\mathcal{L}(R_{n+1,k-1})) < \lambda_2(\mathcal{L}(R_{n,k}))$ for $n \geq k$.

■

Example 3.4
Eigenvalues of $\mathcal{L}(R_{3,4})$ are $\{2., 1.89602, 1.89412, 1.64606, 1.30283, 1.26594, 1.11107, 0.888932, 0.734061, 0.697172, 0.353942, 0.105883, 0.103984, 0.\}$ and $\lambda_2(\mathcal{L}(R_{3,4}))$ is 0.103984. Eigenvalues of $\mathcal{L}(R_{2,5})$ are $\{2., 1.90145, 1.7937, 1.64746, 1.32451, 1.24638, 1., 1., 0.753623, 0.67549, 0.352543, 0.206297, 0.0985536, 0.\}$ and its $\lambda_2(\mathcal{L}(R_{2,5}))$ is 0.0985536. That is $\lambda_2(\mathcal{L}(R_{2,5})) < \lambda_2(\mathcal{L}(R_{3,4}))$. Similarly, eigenvalues of $\mathcal{L}(R_{3,3})$ is $\{2., 1.89416, 1.85239, 1.5, 1.29156, 1., 1., 0.708438, 0.5, 0.147607, 0.105836, 0.\}$ and $\lambda_2(\mathcal{L}(R_{3,3}))$ is 0.105836. Eigenvalues of $\mathcal{L}(R_{4,2})$ is $\{2., 1.93653, 1.85221, 1.5, 1.41765, 1., 1., 0.582351, 0.5, 0.147788, 0.0634731, 0.\}$ and $\lambda_2(\mathcal{L}(R_{4,2}))$ is 0.0634731. That is $\lambda_2(\mathcal{L}(R_{4,2})) < \lambda_2(\mathcal{L}(R_{3,3}))$.

Proposition 3.16 ([9])
If $G = (V(G), E(G)$ be a graph with $|V(G)| = n$ and more than $n/2$ of the vertices are connected to every other vertex then $n/(n-1)$ is an eigenvalue of $\mathcal{L}(G)$.

■

Example 3.5
The Figure 13 shows a graph with 6 vertices. 4 vertices are connected to every other and the eigenvalues are $\{1.4, 1.2, 1.2, 1.2, 1., 0.\}$. Hence $\frac{n}{n-1} = 1.2$ is an eigenvalue by the Proposition 3.16.

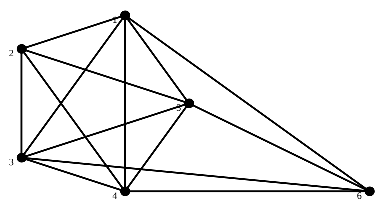


Figure 13: Graph which has more than half of vertices connected to each other.

Lemma 3.11
The normalized Laplacian of K_n has an eigenvalue 0 with multiplicity 1 and $\dfrac{n}{n-1}$ with multiplicity $n-1$.

(Proof) Let x be any vector orthogonal to the $D^{1/2}\vec{1}$. Consider the first row expansion of $\mathcal{L}(G)x = \lambda x$.

$$\begin{aligned} x_1 - \sum_{i=2}^{n} \frac{x_i}{n-1} &= \lambda x_1 \\ x_1 - \frac{1}{n-1}(\sum_{i=1}^{n} x_i - x_1) &= \lambda x_1 \\ x_1 - \frac{1}{n-1}\sum_{i=1}^{n} x_i + \frac{x_1}{n-1} &= \lambda x_1 \\ \frac{n}{n-1} &= \lambda \end{aligned}$$

Thus, x is an eigenvector with an eigenvalue $\dfrac{n}{n-1}$. ■

3.2.6 Normalized eigenvalues of elementary graphs

Here are some examples of special graphs and their eigenvalues [10].

1. *Eigenvalues of $\mathcal{L}(P_n)$ are $1 - \cos\dfrac{\pi k}{n-1}$ for $k = 0, \ldots, n-1$.*

2. *Eigenvalues of $\mathcal{L}(C_n)$ are $1 - \cos\dfrac{2\pi k}{n}$ for $k = 0, \ldots, n-1$.*

3. *Eigenvalues of $\mathcal{L}(K_n)$ are 0 and $\dfrac{n}{n-1}$ with multiplicity $n-1$.*

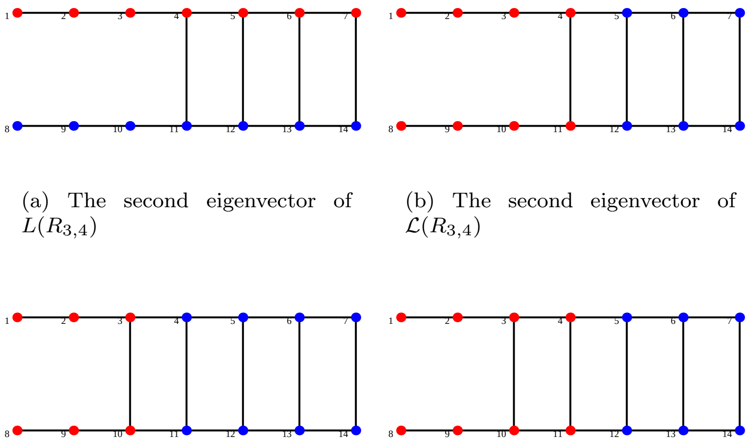
4. *Eigenvalues of complete bipartite graph $\mathcal{L}(K_{m,n})$ are 0,1(with multiplicity $m+n-2$), and 2.*

5. *Eigenvalues of Star graph $\mathcal{L}(S_n)$ are 0, 1(with multiplicity $n-2$), and 2.*

6. *For the n- cube Q_n on 2^n vertices, the eigenvalues are $\dfrac{2k}{n}$(with multiplicity $\binom{n}{k}$)for $k = 0, \ldots, n$.*

3.2.7 Sign patterns of difference and normalized Laplacian eigenvectors

Sign patterns of the second eigenvector of difference Laplacian and normalized Laplacian are not always same. The Figure 14 shows some examples, where these two produce different clusters. In the Figure 14(b), vertices $\{1, 2, 3, 4, 8, 9, 10, 11\}$ are belong to one group and $\{5, 6, 7, 12, 13, 14\}$ are belong to other. This makes the second eigenvector of Laplacian even under the automorphism $\phi(v_i) = v_{i+n+k}$ for $i = 1, \ldots, n+k$. But the second eigenvector of difference Laplacian is odd under the same automorphism as shown in the Figure 14(a). When we look at the clustering on the Figure 14(c), *vertices* $\{1, 2, 3, 8, 9, 10\}$ *are belong to the first group and* $\{4, 5, 6, 7, 11, 12, 13, 14\}$ *are belong to the second group. In the Figure 14(d), vertices* $\{1, 2, 3, 4, 8, 9, 10, 11\}$ *are belong to the first group and remaining vertices are belong to the second group. We can find many counter examples, where the second eigenvector of Laplacian and normalized Laplacian have different sign patterns.*



(a) The second eigenvector of $L(R_{3,4})$

(b) The second eigenvector of $\mathcal{L}(R_{3,4})$

(c) The second eigenvector of $L(R_{2,5})$

(d) The second eigenvector of $\mathcal{L}(R_{2,5})$

Figure 14: Sign patterns of the second eigenvector of Laplacian and normalized Laplacian of $R_{n,k}$.

In this section we analyze the signless Laplacian and derive some upper bounds.

3.3 Signless Laplacian

Signless Laplacian matrix of unweighted graph G *is denoted by* $SL(G) = D + A$. *The eigenvalues of* $SL(G)$ *will be called the signless eigenvalues. For a connected graph* G, *it is well known that* $SL(G)$ *is a positive semidefinite matrix, that is, all its eigenvalues are nonnegative. Furthermore, by the Perron-Frobenius theorem, the largest eigenvalue* $\mu(G)$ *of* $SL(G)$ *is simple and there is a unique positive unit eigenvector* $X = (x_1, \ldots, x_n)^T$. *This eigenvector is referred as the Perron vector of* $SL(G)$.

Example 3.6
Eigenvalues of signless Laplacian of cycle C_6 *are* $\{4, 3, 3, 1, 1, 0\}$ *and it is clear that its largest eigenvalue is simple. Eigenvectors of* $SL(C_6)$ *are* $\{(1, 1, 1, 1, 1, 1), (1, 0, -1, -1, 0, 1), (-1, -1, 0, 1, 1, 0), (-1, 0, 1, -1, 0, 1), (-1, 1, 0, -1, 1, 0), (-1, 1, -1, 1, -1, 1)\}$ *and the largest eigenvector is a positive constant vector.*

Remarks. *Let* G *be a simple connected graph. Then* $SL(G)$ *is an irreducible nonnegative matrix.*

Proposition 3.17
Let A be an irreducible non-negative $n \times n$ matrix with spectral radius $\rho(A) = r$, where r is a positive real number and it is an eigenvalue of the matrix A called the **Perron-Frobenius eigenvalue**. *Then the following statements hold.*

1. *The Perron-Frobenius eigenvalue r is simple.*
2. *Both right and left eigenspaces associated with r are one-dimensional.*
3. *The matrix A has a left eigenvector v with an eigenvalue r whose components are all positive.*
4. *Likewise, matrix A has a right eigenvector w with an eigenvalue r whose components are all positive.*
5. *The only eigenvectors whose components are all positive are those associated with the eigenvalue r.*

3.3.1 Signless Laplacian eigenvalues of some graphs

Signless Laplacian eigenvalues of path and cycles can be easily derived from the difference Laplacian eigenvalues.

Proposition 3.18
For cycles C_n, signless Laplacian eigenvalues are $2 + 2\cos(\frac{2k\pi}{n}), k = 0, \ldots, n-1$.

$\blacksquare$

Proposition 3.19
For paths P_n, signless eigenvalues are $2 + 2\cos(\frac{k\pi}{n}), k = 1, \ldots, n$.

$\blacksquare$

Proposition 3.20
Let K_n be the complete graph. Then signless Laplacian eigenvalues are $2(n-1)$ and $n-2$ with the multiplicity $(n-1)$ while difference Laplacian eigenvalues are 0 and n with multiplicity $n-1$.

$\blacksquare$

(Proof) Let SL be the signless Laplacian matrix, $k = (n-1)$ be the degree of the graph and I the identity matrix. Then

$$
\begin{aligned}
|SL - \mu I| = \det \begin{bmatrix} k-\mu & 1 & \cdots & \cdots & 1 \\ 1 & k-\mu & & & 1 \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 1 & 1 & & & k-\mu \end{bmatrix} &= 0 \\
(k-\mu+(n-1)) \det \begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ 1 & k-\mu & \dots & \dots & 1 \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 1 & 1 & \dots & \dots & k-\mu \end{bmatrix} &= 0 \\
(k-\mu+(n-1)) \det \begin{bmatrix} 1 & 1 & \dots & \dots & 1 \\ 0 & 1-k+\mu & & & 0 \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & \dots & \dots & 1-k+\mu \end{bmatrix} &= 0 \\
(k-\mu+(n-1))(1-k+\mu)(n-1) &= 0
\end{aligned}
$$

This implies that $\mu = k+n-1$ or $\mu = k-1$ with multiplicity $(n-1)$. That is the eigenvalues are $2(n-1)$ with multiplicity 1 and $(n-2)$ with multiplicity $(n-1)$. ■

3.3.2 Properties of signless Laplacian

Proposition 3.21
Quadratic form of signless Laplacian can be written as

$$
\begin{aligned}
(SL(G)f)_i &= \sum_{i=1}^{n}\sum_{j=1}^{n}(f_i+f_j)w_{ij} \\
f^T SL(G) f &= \sum_{i=1}^{n}\sum_{j=1}^{n}(f_i+f_j)^2 w_{ij} \\
\mu_2 = \min \frac{f^T SL(G) f}{f^T f} &= \frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(f_i+f_j)^2 w_{ij}}{2\sum_i f_i^2}.
\end{aligned}
$$

Note. *For each edge $(i,j) \in E(G)$, if we assign $f_i = -f_j$ then $\mu_2(SL(G)) = 0$ and this lead to the following proposition.*

Proposition 3.22
The least eigenvalue of the signless Laplacian of a connected graph is equal to 0 if and only if the graph is bipartite and 0 is a simple eigenvalue. ■

Corollary 3.14 ([51])
For any graph, the multiplicity of 0 as an eigenvalue of the signless Laplacian is equal to the number of bipartite components.

■

Proposition 3.23 ([33])
The characteristic polynomial of the signless Laplacian matrix is equal to the characteristic polynomial of the difference Laplacian if and only if the graph is bipartite.

Zhongxun Zhu 2011, [51] studied the spectral radius of signless Laplacian and determine the graph with the largest signless Laplacian spectral radius in bicyclic graphs with girth n.

Lemma 3.12 ([49])
Let $G = (V(G), E(G))$ be a connected simple graph with $(u, v_i) \in E(G)$ and $(w, v_i) \notin E(G)$ for $i = 1, \ldots, k$. Let $G' = (V(G'), E(G'))$ be a new graph from G by deleting edges (u, v_i) and adding edges (w, v_i) for $i = 1, \ldots, k$. Let f be a Perron vector of $SL(G)$. If $f_w \geq f_u$, then $\mu(G) < \mu(G')$.

(Proof) Let S be the set of all unit vectors in $\Re^n$. By the Rayleigh quotient of $SL(G)$ on vectors g on $V(G)$, $\mu(G) = \max\limits_{g\in S} g^T SL(G)g = \max\limits_{g\in S} \dfrac{\sum_{i=1}^n \sum_{j=1}^n (g_i+g_j)^2}{2} = \dfrac{\sum_{i=1}^n \sum_{j=1}^n (f_i+f_j)^2}{2}$.
Moreover $\mu(G') - \mu(G) = \dfrac{\sum_{i=1}^n \sum_{j=1_{i,j\in V(G')}}^n (f_i+f_j)^2}{2} - \dfrac{\sum_{i=1}^n \sum_{j=1_{i,j\in V(G)}}^n (f_i+f_j)^2}{2}$.
This is equal to $\dfrac{\sum_{i=1}^n (f_{v_i}+f_w)^2}{2} - \dfrac{\sum_{i=1}^n (f_{v_i}+f_u)^2}{2} = \dfrac{\sum_{i=1}^k (f_w^2 - f_u^2 + 2f_{v_i}f_w - 2f_{v_i}f_u)}{2} = \dfrac{(f_w - f_u)\sum_{i=1}^k f_w + f_u + 2f_{v_i}}{2} \geq 0$. Hence $\mu(G') \geq \mu(G)$.

If $\mu(G) = \mu(G')$ then f is the Perron vector of G'. Hence $SL(G)f = \mu(G)f$ and $SL(G')f = \mu(G')f$. By expanding the formula corresponding to the vertex u we have, $\mu(G)f_u = d_u(G)f_u + \sum_{i=1}^k f_{v_i} + \sum_{m\neq v_i,(m,u)\in E(G)} f_m$.
Similarly, $\mu(G')f_u = d_u(G')f_u + \sum_{j\neq v_i,(j,u)\in E(G')} f_j$. Therefore $\mu(G)f_u - \mu(G')f_u = d_u(G)f_u - d_u(G')f_u + \sum_{i=1}^k f_{v_i} = 0$. Then $\sum_{i=1}^k f_{v_i} = 0$ by $d_u(G) > d_u(G')$. That is impossible and hence $\mu(G') \neq \mu(G)$ and we have $\mu(G') > \mu(G)$. ■

Lemma 3.13 (Zhang [49])
Let $G = (V(G), E(G))$ be a connected simple graph with $(v_1, u_1), (v_2, u_2) \in E(G)$ and $(v_1, v_2), (u_1, u_2) \notin E(G)$. Let $G' = (V(G'), E(G'))$ be a new graph from G by deleting edges $(v_1, u_1), (v_2, u_2)$ and adding edges (v_1, v_2) and (u_1, u_2). Let f be a Perron vector of G. If $f_{v_1} \geq f_{u_2}$ and $f_{v_2} \geq f_{u_1}$, then $\mu_{G'} \geq \mu_G$. Moreover, if one of the two inequalities is strict then $\mu(G') > \mu(G)$.

(Proof) Since f is a Perron vector of G, $\mu(G) = \max\limits_{g\in S} g^T SL(G)g = \max\limits_{g\in S} \dfrac{\sum_{i=1}^n \sum_{j=1}^n (g_i+g_j)^2}{2} = \dfrac{\sum_{i=1}^n \sum_{j=1}^n (f_i+f_j)^2}{2}$. Moreover, $\mu(G') - \mu(G) = \dfrac{\sum_{i=1}^n \sum_{j=1_{i,j\in V(G')}}^2 (f_i+f_j)^2}{2} - \dfrac{\sum_{i=1}^n \sum_{j=1_{i,j\in V(G)(f_i+f_j)^2}}^n}{2} = (f_{v_2} - f_{u_1})(f_{v_1} - f_{u_2}) \geq 0$. Hence $\mu(G') \geq \mu(G)$.

If $\mu(G) = \mu(G')$ then f is the Perron vector of G' and we have $SL(G)f = \mu(G)f$ and $SL(G')f = \mu(G')f$. Expanding the equation corresponding to v_1, We have $\mu(G)f_{v_1} = d_{v_1}(G)f_{v_1} + f_{u_1} + \sum_{(v_1,j)\in\{E(G)\cap E(G')\}} f_j$.

Similarly, $\mu(G')f_{v_1} = d_{v_1}(G')f_{v_1} + f_{v_2} + \sum_{(v_1,j)\in\{E(G)\cap E(G')\}} f_j$. Hence $f_{u_1} = f_{v_2}$ by $d_{v_1}(G) = d_{v_1}(G')$.

Similarly, we can show that $f_{v_1} = f_{u_2}$. ■

3.4 The eigenvalues and the eigenvectors of paths and cycles

In this section, we derive formula for the eigenvalues and eigenvectors of cycles and paths using circulant matrices and give an alternate proof for the eigenvalues of adjacency matrix of cycles and paths using Chebyshev polynomials.

3.4.1 Circulant matrices and eigenvalues of cycles and paths

Let $\omega_n = \mathbf{e}^{-\frac{2\pi}{n}\mathbf{i}} = \cos\frac{2\pi}{n} + \mathbf{i}\sin\frac{2\pi}{n}$ be a primitive n-th root of unity.

Definition 3.1
A circulant matrix $C = (c_{ij})$ is a matrix having a form $c_{ij} = c_{(j-i) \mod n}$.

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

Proposition 3.24
Let $C = (c_{ij})$ be a circulant matrix and $c_{ij} = c_{(j-i) \mod n}$. For $k = 0, \ldots, n-1$, we have

$$C\mathbf{u}_k = \lambda_k \mathbf{u}_k,$$

where $\lambda_k = \sum_{j=0}^{n-1} c_j (\omega_n^k)^j$, $\mathbf{u}_k = (u_{ki})$ and $u_{ki} = (\omega_n^k)^i = \cos\frac{2k\pi i}{n} + \mathbf{i}\sin\frac{2k\pi i}{n}$.

(Proof)

$$
\begin{aligned}
(C\mathbf{u}_k)_i &= \sum_{j=0}^{n-1} c_{ij} u_{kj} \\
&= \sum_{j=0}^{n-1} c_{(j-i) \mod n} (\omega_n^k)^j \\
&= (\omega_n^k)^i \sum_{j=0}^{n-1} c_{(j-i) \mod n} (\omega_n^k)^{j-i} \\
&= (\omega_n^k)^i \sum_{j=0}^{n-1} c_j (\omega_n^k)^j \\
&= \lambda_k u_{ki} \\
&= (\lambda_k \mathbf{u}_k)_i.
\end{aligned}
$$

■

Proposition 3.25

1. *Eigenvalues of the adjacency matrix of C_n is given by $\lambda_k = 2\cos(\frac{2k\pi}{n})$,*

2. *Eigenvalues of the difference Laplacian matrix of C_n is given by $\lambda_k = 2 - 2\cos(\frac{2k\pi}{n})$,*

3. *Eigenvalues of the normalized Laplacian matrix of C_n is given by $\lambda_k = 1 - \cos(\frac{2k}{n}\pi)$, and*

4. *Eigenvalues of the signless Laplacian matrix of C_n is given by $\lambda_k = 2 + 2\cos(\frac{2k}{n}\pi)$, where $k = (0, \ldots, n-1)$.*

(Proof)

1. *Let A be an adjacency matrix of a cycle graph with n vertices. That is $A = (c_{ij}) = c_{(j-i) \mod n}$ and $c_0 = 0$, $c_1 = c_{n-1} = 1$ and $c_i = 0$ for $i = 2, \ldots, n-2$.*

$$
\begin{aligned}
\lambda_k &= (\omega_n^k)^1 + (\omega_n^k)^{n-1} \\
&= (\omega_n^k)^1 + (\omega_n^k)^{-1} \\
&= 2\cos(\frac{2k\pi}{n}).
\end{aligned}
$$

■

2. *Let $L(C_n)$ be the Laplacian matrix of cycle graph with n vertices. That is $L(C_n) = (c_{ij}) = c_{(j-i) \mod n}$ and $c_0 = 2$, $c_1 = c_{n-1} = -1$ and $c_i = 0$ for $i = 2, \ldots, n-2$.*

$$
\begin{aligned}
\lambda_k &= 2 - (\omega_n^k)^1 - (\omega_n^k)^{n-1} \\
&= 2 - ((\omega_n^k)^1 + (\omega_n^k)^{-1}) \\
&= 2 - 2\cos(\frac{2k\pi}{n}).
\end{aligned}
$$

■

3. Let $\mathcal{L}(C_n)$ be the normalized Laplacian matrix of cycle graph with n vertices. That is $\mathcal{L}(C_n) = (c_{ij}) = c_{(j-i) \mod n}$ and $c_0 = 1$, $c_1 = c_{n-1} = -\frac{1}{2}$ and $c_i = 0$ for $i = 2, \ldots, n-2$.

$$\begin{aligned}\lambda_k &= 1 - \frac{1}{2}(\omega_n^k)^1 - \frac{1}{2}(\omega_n^k)^{n-1}\\ &= 1 - \frac{1}{2}((\omega_n^k)^1 + (\omega_n^k)^{-1})\\ &= 1 - \cos(\frac{2k\pi}{n}).\end{aligned}$$

■

4. Let $SL(C_n)$ be the signless Laplacian matrix of cycle graph with n vertices. That is $SL(C_n) = (c_{ij}) = c_{(j-i) \mod n}$ and $c_0 = 2$, $c_1 = c_{n-1} = 1$ and $c_i = 0$ for $i = 2, \ldots, n-2$.

$$\begin{aligned}\lambda_k &= 2 + (\omega_n^k)^1 - (\omega_n^k)^{n-1}\\ &= 2 + ((\omega_n^k)^1 + (\omega_n^k)^{-1})\\ &= 2 + 2\cos(\frac{2k\pi}{n}).\end{aligned}$$

■

Proposition 3.26
Let $\lambda_k (0 \leq k \leq n-1)$ be the k^{th} eigenvalue of an adjacency matrix of C_n. Then $\lambda_k = \lambda_{n-k}$.

(Proof) Eigenvalues of the adjacency matrix of cycle is given by $\lambda_k = 2\cos(\frac{2k\pi}{n})$, where $k = 0, \ldots, n-1$.

$$\begin{aligned}\lambda_0 &= 2,\\ \lambda_1 &= 2\cos(\frac{2\pi}{n}),\\ \lambda_2 &= 2\cos(\frac{4\pi}{n}),\\ &\vdots\\ \lambda_{n-2} &= 2\cos(\frac{4\pi}{n}),\\ \lambda_{n-1} &= 2\cos(\frac{2\pi}{n}).\end{aligned} \tag{3.4.1}$$

This shows that $\lambda_k = \lambda_{n-k}$ for $k = 1, \ldots, n-1$. ■

Proposition 3.27

1. *The eigenvalues of an adjacency matrix of a path graph P_n are given by* $\lambda_k(A(P_n)) = 2\cos(\frac{(k+1)\pi}{n+1}), (k = 0,\dots,n-1)$ *and an eigenvector* $\mathbf{u_k}$ *is given by* $(u_{ki}) = \sin\frac{(i+1)(k+1)\pi}{n+1}, (i = 0,\dots,n-1)$ *and* $(k = 0,\dots,n-1)$.

2. *The eigenvalues of difference Laplacian matrix of P_n are given by* $\lambda_k(L(P_n)) = 2 - 2\cos(\frac{k\pi}{n})$, $(k = 0,\dots,n-1)$ *and its eigenvector* $\mathbf{u_k}$ *is given by* $(u_{ki}) = \cos\left(\frac{(2i+1)k\pi}{2n}\right)$ $(i = 0,\dots,n-1)$.

3. *The eigenvalues of normalized Laplacian matrix of a path P_n are given by* $\lambda_k(\mathcal{L}(P_n)) = 1 - \cos(\frac{k\pi}{n-1})$ $(k = 0,\dots,n-1)$ *and its eigenvector* $\mathbf{u_k}$ *is given by*

$$u_{ki} = \begin{cases} \sqrt{2}\cos\left(\frac{2i\pi k}{2n-2}\right) & i = 1,\dots,n-2, \\ \cos(\frac{2i\pi k}{2n-2}) & i = 0 \text{ and } i = n-1. \end{cases}$$

4. *The eigenvalues of signless Laplacian matrix of P_n are given by* $\lambda_k(SL(P_n)) = 2 + 2\cos(\frac{(k+1)\pi}{n})$, $(k = 0,\dots,n-1)$ *and its eigenvector* $\mathbf{u_k}$ *is given by* $(u_{ki}) = \sin(\frac{(2i+1)k\pi}{2n}), (i = 0,\dots,n-1)$.

(Proof)

1. *Let* $\mathbf{u} = (u_i), (i = 0,\dots,n-1)$ *be an eigenvector for an eigenvalue λ of path P_n. Then, we can write*

$$P_n\mathbf{u} = \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 \\ 1 & 0 & 1 & 0 & & \vdots \\ \vdots & 1 & 0 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 1 \\ 0 & 0 & \cdots & \cdots & 1 & 0 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{n-1} \end{pmatrix} = \lambda\mathbf{u}.$$

Then we have the following equations:

$$\begin{aligned} u_1 &= \lambda u_0, \\ u_0 + u_2 &= \lambda u_1, \\ u_1 + u_3 &= \lambda u_2, \\ &\vdots \\ u_{n-2} &= \lambda u_{n-1}. \end{aligned} \tag{3.4.2}$$

Let $\mathbf{u'} = (u'_i), (i = 0,\dots,2n+1)$ *be an eigenvector of C_{2n+2}, where* $(u'_i) = \sin(\frac{2(i+1)(k+1)\pi}{2n+2}), (i = 0,\dots,2n+1)$ *and* $(k = 0,\dots,2n+1)$. *The eigenvalues of an ad-*

jacency matrix of a cycle C_{2n+2} are $\lambda_k = 2\cos(\frac{(k+1)\pi}{n+1}), (k = 0, \ldots, 2n+1)$. We note that $u'_n = u'_{2n+1} = 0$. Hence we can write the equation $C_{2n+2}\mathbf{u'} = \lambda_k \mathbf{u'}$ as

$$\begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 1 \\ 1 & 0 & 1 & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & & & & \vdots \\ \vdots & & 1 & 0 & 1 & & & \vdots \\ \vdots & & & 1 & 0 & 1 & & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & & 1 & 0 & 1 \\ 1 & 0 & \cdots & \cdots & \cdots & \cdots & 1 & 0 \end{pmatrix} \begin{pmatrix} u'_0 \\ \vdots \\ u'_{n-1} \\ 0 \\ u'_{n+1} \\ \vdots \\ u'_{2n} \\ 0 \end{pmatrix} = \lambda_k \mathbf{u'}.$$

Then we have the following equations:

$$\begin{aligned} u'_1 &= \lambda_k u'_0, \\ u'_0 + u'_2 &= \lambda_k u'_1, \\ &\vdots \\ u'_{n-2} &= \lambda_k u'_{n-1}. \end{aligned}$$

Comparing the Equation 3.4.1 and the Equation 3.4.2, we have $P_n\mathbf{u} = \lambda_k\mathbf{u}$, where $\mathbf{u} = (u'_i)(i = 0, \ldots, n-1)$. That is $\lambda_k, (k = 0, \ldots, n-1)$ are eigenvalues of P_n and $\mathbf{u}$ is an eigenvector of λ_k. Since $\lambda_i \neq \lambda_j$ for ($i \neq j$ and $0 \leq i, j \leq n-1$), we have n different eigenvalues of P_n and that is the complete set of eigenvalues of P_n.

2. *Let $\mathbf{u} = (u_i), (i = 0, \ldots, n-1)$ be an eigenvector for an eigenvalue λ of difference Laplacian matrix $L(P_n)$. Then we can write the equation $L(P_n)\mathbf{u} = \lambda\mathbf{u}$ as*

$$\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & & 0 \\ \vdots & -1 & 2 & -1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & -1 & 2 & -1 \\ 0 & 0 & \cdots & \cdots & -1 & 2 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \lambda\mathbf{u}.$$

Then we have the following equations.

$$\begin{aligned} u_0 - u_1 &= \lambda u_0, \\ -u_0 + 2u_1 - u_2 &= \lambda u_1, \\ &\vdots \\ -u_{n-2} + u_{n-1} &= \lambda u_{n-1}. \end{aligned} \tag{3.4.3}$$

Let $\mathbf{u}' = (u'_i), (i = 0, \ldots, 2n-1)$ *be an eigenvector of difference Laplacian matrix of* C_{2n}*, where* $(\mathbf{u}'_i) = \cos\left(\dfrac{(2i+1)k\pi}{2n}\right), (i = 0, \ldots, 2n-1)$ *and* $(k = 0, \ldots, 2n-1)$*. The eigenvalues of* $L(C_{2n})$ *are* $\lambda_k = 2 - 2\cos(\dfrac{k\pi}{n}), (k = 0, \ldots, 2n-1)$*. We note that* $u'_0 = u'_{2n-1}, u'_1 = u'_{2n-2}, \ldots, u'_{n-1} = u'_n$*.*
Then we can write the equation $L(C_{2n})\mathbf{u}' = \lambda_k \mathbf{u}'$ *as*

$$\begin{pmatrix} 2 & -1 & 0 & \cdots & \cdots & -1 \\ -1 & 2 & -1 & 0 & & 0 \\ \vdots & -1 & 2 & -1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & -1 & 2 & -1 \\ -1 & 0 & \cdots & \cdots & -1 & 2 \end{pmatrix} \begin{pmatrix} u'_0 \\ u'_1 \\ \vdots \\ \vdots \\ u'_{2n-2} \\ u'_{2n-1} \end{pmatrix} = \lambda_k \mathbf{u}'.$$

$$\begin{aligned} 2u'_0 - u'_1 - u'_{2n-1} &= u'_0 - u'_1 = \lambda_k u'_0, \\ -u'_0 + 2u'_1 - u'_2 &= \lambda_k u'_1, \\ &\vdots \\ -u'_{n-2} + 2u'_{n-1} - u'_n &= -u'_{n-2} + u'_{n-1} = \lambda_k u'_{n-1}. \end{aligned} \tag{3.4.4}$$

Comparing the Equation 3.4.3 and the Equation 3.4.4, we have $P_n\mathbf{u} = \lambda_k \mathbf{u}$*, where* $\mathbf{u} = (u'_i), (i = 0, \ldots, n-1)$*. That is* $\lambda_k, (k = 0, \ldots, n-1)$ *are eigenvalues of* P_n *and* $\mathbf{u}$ *is an eigenvector of* λ_k*. Since* $\lambda_i \neq \lambda_j$ *for* $(i \neq j$ *and* $0 \leq i, j \leq n-1)$*, we have* n *different eigenvalues of* P_n *and that is the complete set of eigenvalues of* P_n*.*

3. *Let* $\mathbf{u} = (u_i), (i = 0, \ldots, n-1)$ *be an eigenvector for an eigenvalue* λ *of normalized Laplacian matrix of path* P_n*. Then we can write the equation* $\mathcal{L}(P_n)\mathbf{u} = \lambda \mathbf{u}$ *as*

$$\begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{2} & 0 & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & -\frac{1}{2} & 1 & -\frac{1}{\sqrt{2}} \\ \vdots & \cdots & \cdots & \cdots & -\frac{1}{\sqrt{2}} & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \lambda \mathbf{u}.$$

By expanding this we have the following equations.

$$\begin{aligned}
u_0 - \frac{1}{\sqrt{2}}u_1 &= \lambda u_0, \\
-\frac{1}{\sqrt{2}}u_0 + u_1 - \frac{1}{2}u_2 &= \lambda u_1, \\
&\vdots \\
-\frac{1}{2}u_{n-3} + u_{n-2} - \frac{1}{\sqrt{2}}u_{n-1} &= \lambda u_{n-2}, \\
-\frac{1}{\sqrt{2}}u_{n-2} + u_{n-1} &= \lambda u_{n-1}.
\end{aligned} \tag{3.4.5}$$

Let $\mathbf{u}' = (u_i'), (i = 0, \ldots, 2n-3)$ *be an eigenvector of normalized Laplacian matrix of* C_{2n-2}*, where* $(u_i') = \cos(\frac{2ik\pi}{2n-2}), (i = 0, \ldots, 2n-3)$ *and* $\lambda_k = 1 - \cos(\frac{2k\pi}{2n-2}), (k = 0, \ldots, 2n-3)$ *be its eigenvalue. We note that* $u_1' = u_{2n-3}', u_2' = u_{2n-4}', \ldots, u_{n-2}' = u_n'$*. Then we multiply each of these values by* $\frac{1}{\sqrt{2}}$ *and obtain the vector,* $u_0', \frac{1}{\sqrt{2}}u_1', \frac{1}{\sqrt{2}}u_2', \ldots, \frac{1}{\sqrt{2}}u_{n-2}', u_{n-1}', \frac{1}{\sqrt{2}}u_n', \ldots, \frac{1}{\sqrt{2}}u_{2n-3}'$*. We can write* $\mathcal{L}(C_{2n-2})\mathbf{u}' = \lambda_k \mathbf{u}'$ *as*

$$\begin{pmatrix}
1 & -\frac{1}{2} & \cdots & \cdots & \cdots & -\frac{1}{2} \\
-\frac{1}{2} & 1 & -\frac{1}{2} & & & \vdots \\
\vdots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \vdots \\
\vdots & & & -\frac{1}{2} & 1 & -\frac{1}{2} \\
-\frac{1}{2} & \cdots & \cdots & \cdots & -\frac{1}{2} & 1
\end{pmatrix}
\begin{pmatrix}
u_0' \\
\frac{1}{\sqrt{2}}u_1' \\
\vdots \\
u_{n-1}' \\
\vdots \\
\frac{1}{\sqrt{2}}u_{2n-3}'
\end{pmatrix} = \lambda_k \mathbf{u}'.$$

By expanding we have,

$$\begin{aligned}
u_0 - \frac{1}{2}\frac{1}{\sqrt{2}}u_1' - \frac{1}{2}\frac{1}{\sqrt{2}}u_1' &= u_0' - \frac{1}{\sqrt{2}}u_1' = \lambda_k u_0', \\
-\frac{1}{2}u_0' + \frac{1}{\sqrt{2}}u_1' - \frac{1}{2}\frac{1}{\sqrt{2}}u_2' &= \frac{1}{\sqrt{2}}(-\frac{1}{\sqrt{2}}u_0' + u_1' - \frac{1}{2}u_2') = \lambda_k(\frac{1}{\sqrt{2}}u_1'), \\
&\vdots \\
-\frac{1}{2}\frac{1}{\sqrt{2}}u_{n-3}' + \frac{1}{\sqrt{2}}u_{n-2}' - \frac{1}{2}u_{n-1}' &= \lambda_k(\frac{1}{\sqrt{2}}u_{n-2}'), \\
-\frac{1}{2}\frac{1}{\sqrt{2}}u_{n-2}' + u_{n-1}' - \frac{1}{2}\frac{1}{\sqrt{2}}u_{n-2}' &= -\frac{1}{\sqrt{2}}u_{n-2}' + u_{n-1}' = \lambda_k u_{n-1}'.
\end{aligned} \tag{3.4.6}$$

Comparing the Equation 3.4.5 and the Equation 3.4.6, we have $P_n\mathbf{u} = \lambda_k\mathbf{u}$*, where* $\mathbf{u} = (u_0', \sqrt{2}u_1', \ldots, \sqrt{2}u_{n-2}', u_{n-1}')$*. That is* $\lambda_k, (k = 0, \ldots, n-1)$ *are eigenvalues of* P_n *and* $\mathbf{u}$ *is an eigenvector of* λ_k*. Since* $\lambda_i \neq \lambda_j$ *for* $(i \neq j$ *and* $0 \leq i, j \leq n-1)$*, we have* n *different eigenvalues of* P_n *and that is the complete set of eigenvalues of* P_n*.*

4. Let $\mathbf{u} = (u_i), (i = 0, \ldots, n-1)$ *be an eigenvector for an eigenvalue* λ *of signless Laplacian matrix of path* P_n*. Then we can write the following equation.*

$$SL(P_n)\mathbf{u} = \begin{pmatrix} 1 & 1 & 0 & \cdots & \cdots & 0 \\ 1 & 2 & 1 & 0 & & \vdots \\ \vdots & 1 & 2 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 1 \\ 0 & 0 & \cdots & \cdots & 1 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix} = \lambda \mathbf{u}.$$

$$\begin{aligned} u_0 + u_1 &= \lambda u_0, \\ u_0 + 2u_1 + u_2 &= \lambda u_1, \\ &\vdots \\ u_{n-2} + 2u_{n-1} &= \lambda u_{n-1}. \end{aligned} \tag{3.4.7}$$

Let $\mathbf{u}' = (u'_i), (i = 0, \ldots, 2n-1)$ *be an eigenvector of signless Laplacian matrix of* C_{2n}*, where* $(u'_i) = \sin(\frac{(2i+1)k\pi}{2n}), (i = 0, \ldots, 2n-1)$ *and* $\lambda_k = 2 + 2\cos(\frac{(k+1)\pi}{2n}), (k = 0, \ldots, 2n-1)$ *be its eigenvalue. We note that* $u'_0 = -u'_{2n-1}, u'_1 = -u'_{2n-2}, \ldots, u'_{n-1} = -u'_n$*. Then we can write the equation* $SL(C_{2n})\mathbf{u}' = \lambda_k \mathbf{u}'$ *as*

$$\begin{pmatrix} 2 & 1 & 0 & \cdots & \cdots & 1 \\ 1 & 2 & 1 & 0 & & 0 \\ \vdots & 1 & 2 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & 1 & 2 & 1 \\ 1 & 0 & \cdots & \cdots & 1 & 2 \end{pmatrix} \begin{pmatrix} u'_0 \\ u'_1 \\ \vdots \\ \vdots \\ u'_{2n-2} \\ u'_{2n-1} \end{pmatrix} = \lambda_k \mathbf{u}'.$$

$$\begin{aligned} 2u'_0 + u'_1 - u'_0 &= u'_0 + u'_1 = \lambda_k u'_0, \\ u'_0 + 2u'_1 + u'_2 &= \lambda_k u'_1, \\ &\vdots \\ u'_{n-2} + 2u'_{n-1} - u'_{n-1} &= u'_{n-2} + u'_{n-1} = \lambda_k u'_{n-1}. \end{aligned} \tag{3.4.8}$$

Comparing the Equation 3.4.7 and the Equation 3.4.8, we have $P_n\mathbf{u} = \lambda_k \mathbf{u}$*, where* $\mathbf{u} = (u'_i), (i = 0, \ldots, n-1)$*. That is* $\lambda_k, (k = 0, \ldots, n-1)$ *are eigenvalues of* P_n *and* $\mathbf{u}$ *is an eigenvector of* λ_k*. Since* $\lambda_i \neq \lambda_j$ *for* $(i \neq j$ *and* $0 \leq i, j \leq n-1)$*, we have* n *different eigenvalues of* P_n *and that is the complete set of signless eigenvalues of* P_n*.*

■

3.4.2 Chebyshev polynomials and eigenvalues of adjacency matrix of paths and cycles

Definition 3.2

Let $T_0(x) = 1$ and $U_0(x) = 0$. For $n \in \mathbf{N}$, $T_n(x)$ and $U_n(x)$ are defined by

$$\begin{pmatrix} T_{n+1}(x) \\ U_{n+1}(x) \end{pmatrix} = \begin{pmatrix} x & x^2-1 \\ 1 & x \end{pmatrix} \begin{pmatrix} T_n(x) \\ U_n(x) \end{pmatrix}.$$

We call $T_n(x)$, the Chebyshev polynomials of the first kind, and $U_n(x)$, the Chebyshev polynomials of the second kind.

Example 3.7

By using the above definition we have,

$$\begin{aligned}
\begin{pmatrix} T_1(x) \\ U_1(x) \end{pmatrix} &= \begin{pmatrix} x & x^2-1 \\ 1 & x \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} x \\ 1 \end{pmatrix}, \\
\begin{pmatrix} T_2(x) \\ U_2(x) \end{pmatrix} &= \begin{pmatrix} x & x^2-1 \\ 1 & x \end{pmatrix} \begin{pmatrix} x \\ 1 \end{pmatrix} = \begin{pmatrix} 2x^2-1 \\ 2x \end{pmatrix}, \\
\begin{pmatrix} T_3(x) \\ U_3(x) \end{pmatrix} &= \begin{pmatrix} x & x^2-1 \\ 1 & x \end{pmatrix} \begin{pmatrix} 2x^2-1 \\ 2x \end{pmatrix} \begin{pmatrix} 4x^3-3x \\ 4x^2-1 \end{pmatrix}.
\end{aligned}$$

Proposition 3.28

$$\begin{aligned}
T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x), \text{ and} \\
U_{n+1}(x) &= 2xU_n(x) - U_{n-1}(x).
\end{aligned}$$

(Proof) Let $A = \begin{pmatrix} x & x^2-1 \\ 1 & x \end{pmatrix}$. By the Cayler-Hamilton theorem, we have $A^2 - 2xA + E = \mathbf{O}$, where E is the identity matrix. By the definition of Chebyshev polynomial we have, $\begin{pmatrix} T_n(x) \\ U_n(x) \end{pmatrix} = A^n \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Then we have,

$$\begin{aligned}
\begin{pmatrix} 0 \\ 0 \end{pmatrix} &= (A^2 - 2xA + E) \begin{pmatrix} T_{n-1}(x) \\ U_{n-1}(x) \end{pmatrix} \\
&= A^2 \begin{pmatrix} T_{n-1}(x) \\ U_{n-1}(x) \end{pmatrix} - 2xA \begin{pmatrix} T_{n-1}(x) \\ U_{n-1}(x) \end{pmatrix} + \begin{pmatrix} T_{n-1}(x) \\ U_{n-1}(x) \end{pmatrix} \\
&= \begin{pmatrix} T_{n+1}(x) - 2xT_n(x) + T_{n-1}(x) \\ U_{n+1}(x) - 2xU_n(x) + U_{n-1}(x) \end{pmatrix}.
\end{aligned}$$

■

Proposition 3.29

$$
\begin{aligned}
T_n(x) &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{2k} (x^2-1)^k x^{n-2k}, \\
U_n(x) &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \binom{n+1}{2k+1} (x^2-1)^k x^{n-2k}.
\end{aligned}
$$

■

Proposition 3.30

$$
\begin{aligned}
\cos n\theta &= T_n(\cos\theta). \\
\sin n\theta &= U_n(\cos\theta)\sin\theta.
\end{aligned}
$$

(Proof)

$$
\begin{aligned}
\cos\theta &= T_1(\cos\theta), \\
\sin\theta &= U_1(\cos\theta)\sin\theta, \\
\cos 2\theta &= 2\cos^2\theta - 1 = T_2(\cos\theta), \\
\sin 2\theta &= 2\sin\theta\cos\theta = U_2(\cos\theta)\sin\theta.
\end{aligned}
$$

Assume $T_{n-1}(\cos\theta) = \cos((n-1)\theta)$ *and* $U_{n-1}(\cos\theta)\sin\theta = \sin((n-1)\theta)$.

$$
\begin{aligned}
\cos n\theta + \mathbf{i}\sin n\theta &= (\cos((n-1)\theta) + \mathbf{i}\sin((n-1)\theta))(\cos\theta + \mathbf{i}\sin\theta) \\
&= (T_{n-1}(\cos\theta) + \mathbf{i}U_{n-1}(\cos\theta)\sin\theta)(\cos\theta + \mathbf{i}\sin\theta) \\
&= (\cos\theta\, T_{n-1}(\cos\theta) - \sin^2\theta\, U_{n-1}(\cos\theta)) + \mathbf{i}(\cos\theta\, U_{n-1}(\cos\theta)\sin\theta + T_{n-1}(\cos\theta)\sin\theta) \\
&= (\cos\theta\, T_{n-1}(\cos\theta) + (\cos^2\theta - 1)U_{n-1}(\cos\theta)) \\
&\qquad + \mathbf{i}(\cos\theta\, U_{n-1}(\cos\theta) + T_{n-1}(\cos\theta))\sin\theta \\
&= T_n(\cos\theta) + \mathbf{i}U_n(\cos\theta)\sin\theta.
\end{aligned}
$$

■

Proposition 3.31
Let $x = \cos\theta$.

$$
\begin{aligned}
T_n(x) = 0 \quad &\Leftrightarrow \quad x = \cos(\frac{(2k+1)\pi}{2n}) \quad (k = 0, \ldots, n). \\
U_n(x) = 0 \quad &\Leftrightarrow \quad x = \cos(\frac{k\pi}{n}) \quad (k = 1, \ldots, n-1).
\end{aligned}
$$

(Proof)

$$\begin{aligned} T_n(x) = 0 &\Rightarrow \cos n\theta = 0 \\ &\Rightarrow n\theta = \frac{2k+1}{2}\pi \\ &\Rightarrow \theta = \frac{2k+1}{2n}\pi. \\ U_n(x) = 0 &\Rightarrow \sin n\theta = 0 \\ &\Rightarrow n\theta = k\pi \\ &\Rightarrow \theta = \frac{k}{n}\pi. \end{aligned}$$

Since the degree of $T_n(x)$ is n, $\cos(\frac{(2k+1)\pi}{2n})$ $(k = 0, \ldots, n)$ are the all solutions of $T_n(x) = 0$. Similarly, since the degree of $U_n(x)$ is $n-1$, $\cos(\frac{k\pi}{n})$ $(k = 1, \ldots, n-1)$ are the all solutions of $U_n(x) = 0$. ■

The determinant of tridiagonal matrices can be represented by using recurrence relations. We consider the tridiagonal matrices with similar diagonal elements. Then we derive formula for eigenvalues of tridiagonal matrices.

3.4.3 Determinant of tridiagonal Matrices

Definition 3.3

A $n \times n$ tridiagonal matrix $A_n = (a_{ij})$ is a matrix which has the form

$$A_n = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ \gamma_1 & \alpha_2 & \beta_2 & \ddots & \vdots \\ 0 & \gamma_2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \alpha_{n-1} & \beta_{n-1} \\ 0 & \cdots & 0 & \gamma_{n-1} & \alpha_n \end{pmatrix}.$$

Proposition 3.32

Let $n \geq 2$, $|A_0| = 1$, and $|A_1| = \alpha_1$. By expanding the tridiagonal matrix, We have

$$|A_n| = \alpha_n |A_{n-1}| - \beta_{n-1}\gamma_{n-1}|A_{n-2}|.$$

Proposition 3.33

Eigenvalues of adjacency matrix of path graph is given by $\lambda_k(A(P_n)) = 2\cos(\frac{k\pi}{n+1})(k = 1, \ldots, n)$.

(Proof) Let P_n be a path graph with n vertices. The matrix $\lambda I - P_n$ is a tridiagonal matrix with $\alpha_i = \lambda$, $\beta_i = \gamma_i = -1$. Let $f_n(\lambda) = |\lambda I - P_n|$. By Proposition 3.32, $f_n(\lambda)$ is defined by $f_n(\lambda) =$

$\lambda f_{n-1}(\lambda) - f_{n-2}(\lambda)$, where $f_0(\lambda) = 1$ and $f_1(\lambda) = \lambda$. Let $g_n(\lambda) = U_{n+1}(\frac{\lambda}{2})$. Since

$$\begin{aligned}
g_0(\lambda) &= U_1(\frac{\lambda}{2}) = 1, \\
g_1(\lambda) &= U_2(\frac{\lambda}{2}) = 2(\frac{\lambda}{2}) = \lambda, and \\
g_n(\lambda) &= U_{n+1}(\frac{\lambda}{2}) \\
&= 2\frac{\lambda}{2}U_n(\frac{\lambda}{2}) - U_{n-1}(\frac{\lambda}{2}) \\
&= \lambda g_{n-1}(\lambda) - g_{n-2}(\lambda),
\end{aligned}$$

we have $f_n(\lambda) = g_n(\lambda) = U_{n+1}(\frac{\lambda}{2})$. That is

$$\begin{aligned}
f_n(\lambda) = 0 &\Leftrightarrow U_{n+1}(\frac{\lambda}{2}) = 0 \\
&\Leftrightarrow \frac{\lambda}{2} = \cos(\frac{k\pi}{n+1}) \ (k = 1, \dots, n) \\
&\Leftrightarrow \lambda = 2\cos(\frac{k\pi}{n+1}) \ (k = 1, \dots, n).
\end{aligned}$$

■

Proposition 3.34
Eigenvalues of adjacency matrix of cycle is given by $\lambda_k(A(C_n)) = 2\cos(\frac{2k\pi}{n})(k = 1, \dots, n)$.

(Proof) Let C_n be a cycle graph with n vertices. The matrix $\lambda I - C_n$ is not a tridiagonal matrix. But we have $|\lambda I - C_n| = 2(T_n(\frac{\lambda}{2}) - 1)$. Since $T_n(x) = 1 \Leftrightarrow \cos n\theta = 1 \Leftrightarrow \theta = \frac{2k\pi}{n}$. We obtain

$$|\lambda I - C_n| = \prod_{k=1}^{n}(\lambda - 2\cos(\frac{2k\pi}{n})).$$

■

Proposition 3.35
Let $P_n = (V_n, E_n)$ be a path graph. If $G = (V_n, E_n \cup \{(v_1, v_1)\}, \{(v_n, v_n)\})$ then the eigenvalues of difference Laplacian matrix of G is given by $\lambda_k = a + 2\cos(\frac{k\pi}{n+1}), (k = 1, \dots, n)$.

(Proof) Let $L(P_n)$ the Laplacian matrix of the path graph with vertex weight a on n vertices. The matrix $\lambda I - L(P_n)$ is a tridiagonal matrix with $\alpha_i = \lambda - a$, $\beta_i = \gamma_i = -1$. Let $f_n(\lambda) = |\lambda I - L(P_n)|$.

Figure 15: Path graph with equal vertex degrees

$f_n(\lambda)$ is defined by $f_n(\lambda) = (\lambda - a)f_{n-1}(\lambda) - f_{n-2}(\lambda)$ where $f_0(\lambda) = 1$ and $f_1(\lambda) = \lambda - a$. Let $g_n(\lambda) = U_{n+1}(\dfrac{\lambda - a}{2})$. Since

$$\begin{aligned}
g_0(\lambda) &= U_1(\frac{\lambda - a}{2}) = 1, \\
g_1(\lambda) &= U_2(\frac{\lambda - a}{2}) = 2(\frac{\lambda - a}{2}) = \lambda - a, and \\
g_n(\lambda) &= U_{n+1}(\frac{\lambda - a}{2}) \\
&= 2\frac{\lambda - a}{2}U_n(\frac{\lambda - a}{2}) - U_{n-1}(\frac{\lambda - a}{2}) \\
&= (\lambda - a)g_{n-1}(\lambda) - g_{n-2}(\lambda),
\end{aligned}$$

we have $f_n(\lambda) = g_n(\lambda) = U_{n+1}(\dfrac{\lambda - a}{2})$. That is

$$\begin{aligned}
f_n(\lambda) = 0 \quad &\Leftrightarrow \quad U_{n+1}(\frac{\lambda - a}{2}) = 0 \\
&\Leftrightarrow \quad \frac{\lambda - a}{2} = \cos(\frac{k\pi}{n+1}) \ (k = 1, \ldots, n) \\
&\Leftrightarrow \quad \lambda = a + 2\cos(\frac{k\pi}{n+1}) \ (k = 1, \ldots, n).
\end{aligned}$$

■

3.5 Conclusion

In this chapter, we discuss three matrices associated with graphs called difference Laplacian, normalized Laplacian and signless Laplacian. We discuss their boundaries using Cheeger constant and isoperimetric number. We also give uniform proofs for the eigenvalues of above 3 matrices of cycles and paths using circulant matrices and give an alternate proof for the eigenvalues of adjacency matrices of paths and cycles using Chebyshev polynomials.

4 Counter examples for $Mcut(G) \neq Lcut(G)$

In this chapter, we give counter example graphs, where spectral clustering methods and minimum normalized cut $Mcut(G)$ produce different clusters on graphs.

4.1 Properties of $Lcut(G)$

Definition 4.1 ($Lcut(G)$)
Let $(U_2)_i, 1 \leq i \leq |V(G)|$ be an eigenvector of the second smallest eigenvalue λ_2 of $\mathcal{L}(G)$. We assume that λ_2 is simple. Then $Lcut(G)$ is defined as $Lcut(G) = Ncut(A_{\lambda_2}, B_{\lambda_2})$, where $A_{\lambda_2} = \{v_i \in V | (U_2)_i \geq 0\}$ and $B_{\lambda_2} = \{v_i \in V | (U_2)_i < 0\}$.

Example 4.1 (Graphs with multiplicity of $\lambda_2 > 1$)
The eigenvalues of cycle C_4 are $\{0, 1, 1, 2\}$ and the eigenvectors corresponding to the second smallest eigenvalue are $\{(0.6396, 0.3015, -0.6396, -0.3015), (0.6396, -0.3015, -0.6396, 0.3015)\}$. Then we have $Lcut(C_4) = 1$. But $\{(0, 1, 0, -1)\}$ is also an eigenvector with the second smallest eigenvalue. Then $Ncut(A, V \setminus A) = 3/4$, where $A = \{1, 2, 3\}$ and $V \setminus A = \{4\}$. Then we have $Lcut(C_4) = 3/4$. This shows the choice of eigenvectors is rather delicate.

Example 4.2 ($Mcut(G)$ and $Lcut(G)$)
The Figure 16 shows some examples, where $Mcut(G) = Lcut(G)$ and $Mcut(G) \neq Lcut(G)$. $Mcut(G) = Lcut(G)$ for the Figure 16(a) and the Figure 16(b). $Mcut(R_{6,4}) \neq Lcut(R_{6,4})$ for the graph $R_{6,4}$ shown in the Figure 16(c) and the Figure 16(d).

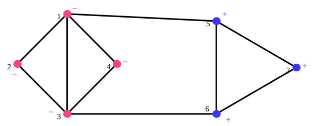
Proposition 4.1 ([46])
Let $A \subseteq V$. If vector $y = (y_1, \ldots, y_n)^T \in \Re^n$ is defined as

$$y = \begin{cases} \sqrt{\frac{vol(V \setminus A)}{vol(A)}} & \text{if } i \in A, \\ -\sqrt{\frac{vol(A)}{vol(V \setminus A)}} & \text{if } i \in (V \setminus A), \end{cases}$$

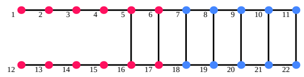
then

1. $y^T L y = vol(V) \cdot Ncut(A, V \setminus A)$,
2. $y^T D y = vol(V)$ *and*
3. $(Dy)^T \vec{1} = 0$.

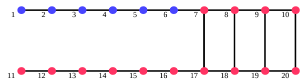
(Proof)



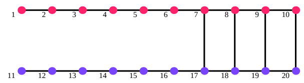
(a) $Lcut(G) = Mcut(G)$



(b) $Lcut(R_{4,7}) = Mcut(R_{4,7})$



(c) $Mcut(R_{6,4})$



(d) $Lcut(R_{6,4})$

Figure 16: $Mcut(G) = Lcut(G)$ and $Mcut(G) \neq Lcut(G)$

1.

$$
\begin{aligned}
y^T L y &= y^T D y - y^T W y \\
&= \sum_{i=1}^{n} d_i y_i^2 - \sum_{i,j} y_i w_{ij} y_j \\
&= \frac{1}{2}\left(\sum_{i=1}^{n} d_i y_i^2 - 2\sum_{i,j} y_i y_j w_{ij} + \sum_{j=1}^{n} d_j y_j^2 \right) \\
&= \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(y_i - y_j)^2.
\end{aligned}
$$

This can be further reduced to,

$$
\begin{aligned}
&= \frac{1}{2}\sum_{i\in A, j\in(V\setminus A)} w_{ij}\left(\sqrt{\frac{vol(V\setminus A)}{vol(A)}}+\sqrt{\frac{vol(A)}{vol(V\setminus A)}}\right)^2 + \\
&\quad \frac{1}{2}\sum_{i\in(V\setminus A), j\in A} w_{ij}\left(-\sqrt{\frac{vol(A)}{vol(V\setminus A)}}-\sqrt{\frac{vol(V\setminus A)}{vol(A)}}\right)^2 \\
&= cut(A, V\setminus A)\left(\frac{vol(A)}{vol(V\setminus A)}+\frac{vol(V\setminus A)}{vol(A)}+2\right) \\
&= cut(A, V\setminus A)\left(\frac{vol(A)+vol(V\setminus A)}{vol(V\setminus A)}+\frac{vol(A)+vol(V\setminus A)}{vol(A)}\right) \\
&= vol(V).Ncut(A, V\setminus A).
\end{aligned}
$$

■

2.

$$
\begin{aligned}
y^T D y &= \sum_{i=1}^{n} d_i y_i^2 \\
&= \sum_{i\in A} d_i y_i^2 + \sum_{i\in(V\setminus A)} d_i y_i^2 \\
&= \sum_{i\in A} d_i\left(\frac{vol(V\setminus A)}{vol(A)}\right) + \sum_{i\in(V\setminus A)} d_i\left(\frac{vol(A)}{vol(V\setminus A)}\right) \\
&= vol(A)\frac{vol(V\setminus A)}{vol(A)} + vol(V\setminus A)\frac{vol(A)}{vol(V\setminus A)} \\
&= vol(V).
\end{aligned}
$$

■

3.

$$
\begin{aligned}
(Dy)^T\vec{1} &= \sum_{i=1}^{n} d_i y_i \\
&= \sum_{i\in A} d_i\sqrt{\frac{vol(V\setminus A)}{vol(A)}} - \sum_{i\in V\setminus A} d_i\sqrt{\frac{vol(V\setminus A)}{vol(A)}} \\
&= vol(A)\sqrt{\frac{vol(V\setminus A)}{vol(A)}} - vol(V\setminus A)\sqrt{\frac{vol(V\setminus A)}{vol(A)}} \\
&= 0.
\end{aligned}
$$

■

Proposition 4.2 (Shi and Malik, 2000[42])
Let $G = (V(G), E(G), w)$ be a graph, where $|V(G)| = n$ and A is a non empty subset of $V(G)$. Let x be an n dimensional indicator vector such that,

$$x_i = \begin{cases} 1 & \text{if } v_i \in A, \\ -1 & \text{otherwise.} \end{cases}$$

Let D be a $(n \times n)$ diagonal matrix of vertex degrees in the diagonal and W be a weighted adjacency matrix of size $(n \times n)$. Then $\min Ncut(x)$ can be written as

$$\min_x Ncut(x) = \min_y \frac{y^T(D-W)y}{y^T Dy}$$

with $y^T D\vec{1} = 0$.

(Proof) [Summary of the proof] If $y \in \Re^n$ is an eigenvector then $Ncut(x)$ can be minimized by solving generalized eigenvalue system,

$$(D - W)y = \lambda Dy. \tag{4.1.1}$$

By substituting $z = D^{\frac{1}{2}}y$, we can rewrite the Equation 4.1.1 as

$$D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}z = \mathcal{L}z = \lambda z, \tag{4.1.2}$$

where z is an eigenvector of $\mathcal{L}$. Then $z_1 = D^{\frac{1}{2}}\vec{1}$ is an eigenvector with an eigenvalue 0. $\mathcal{L}$ is a symmetric positive semidefinite matrix. Hence z_1 is the smallest eigenvector of the Equation 4.1.2 and all the eigenvectors are perpendicular to each other. In particular, the second smallest eigenvector z_2, is perpendicular to the first eigenvector z_1. Then we have $y_1 = \vec{1}$ and $0 = z_2^T z_1 = y_2^T D\vec{1}$, where y_1 is the first eigenvector and y_2 is the second smallest eigenvector of the Equation 4.1.2. Using the property of Rayleigh quotient we obtain,

$$z_2 = arg \cdot min_{z^T z_1 = 0} \frac{z^T D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}z}{z^T z} \tag{4.1.3}$$

and consequently,

$$y_2 = arg \cdot min_{y^T D\vec{1} = 0} \frac{y^T(D-W)y}{y^T Dy}. \tag{4.1.4}$$

Therefore the second smallest eigenvector of the generalized eigensystem (Equation 4.1.1) is a real valued solution to the normalized cut problem[42]. Generalized eigensystem in the the Equation 4.1.1 can be transformed to $D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}x = \lambda x$ by substituting $y = D^{-\frac{1}{2}}x$, where x is an eigenvector of $\mathcal{L}(G) = D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}$. If x is an eigenvector of $\mathcal{L}(G)$ then $D^{-\frac{1}{2}}x$ is an eigenvector for the eigensystem in the Equation 4.1.1. ■

4.2 The graph $R_{n,k}$

Proposition 4.3
Let $U = (u_1, u_2, \ldots, u_{2(n+k)})$ is an eigenvector of $\mathcal{L}(R_{n,k})$ with an eigenvalue λ. If U is an even vector then, $\bar{U}$ is an eigenvector of $\mathcal{L}(P_{n,k})$ with an eigenvalue λ, where $\bar{U} = (u_1, u_2, \ldots, u_{n+k})$.

(Proof) Since U is an even vector then there exists an automorphism ϕ such that $\phi(u_i) = u_{n+k+i}$ for $(i = 1, \ldots, n+k)$. Then we can define U as $U = (u_1, u_2, \ldots, u_{(n+k)}, u_1, u_2, \ldots, u_{(n+k)})$, which can be written as $U = (\bar{U}, \bar{U})$.
Then $\mathcal{L}(R_{n,k})$ can be written as

$$\mathcal{L}(R_{n,k}) = \begin{pmatrix} \mathcal{L}_1 & C \\ C^T & \mathcal{L}_1 \end{pmatrix},$$

where $\mathcal{L}_1$ is the $(n+k)\times(n+k)$ principal sub matrix of $\mathcal{L}(R_{n,k})$ and $C = (c_{ij})$ is the $(n+k)\times(n+k)$ matrix such that

$$c_{ij} = \begin{cases} 1 & \text{if } n+1 \le i \le n+k, \\ 0 & \text{otherwise.} \end{cases}$$

We noticed that $\mathcal{L}_1 + C = \mathcal{L}(P_{n,k})$. If λ is an eigenvalue of $\mathcal{L}(R_{n,k})$ then $\mathcal{L}(R_{n,k})U = \lambda U$ can be written as,

$$\begin{pmatrix} \mathcal{L}_1 & C \\ C^T & \mathcal{L}_1 \end{pmatrix} \begin{pmatrix} \bar{U} \\ \bar{U} \end{pmatrix} = \lambda \begin{pmatrix} \bar{U} \\ \bar{U} \end{pmatrix}$$

This gives

$$\mathcal{L}_1\bar{U} + C\bar{U} \;\; = \;\; \lambda\bar{U}.$$

This can be written as, $(\mathcal{L}_1 + C)\bar{U} = \mathcal{L}(P_{n,k})\bar{U} = \lambda\bar{U}$. Therefore λ is an eigenvalue of $\mathcal{L}(P_{n,k})$ and $\bar{U}$ is an eigenvector. Thus if U is an even vector of $\mathcal{L}(R_{n,k})$ with eigenvalue λ, then $\bar{U}$ is an eigenvector of $\mathcal{L}(P_{n,k})$ with the same eigenvalue. Converse of this proposition also holds. ■

Proposition 4.4
Let $U = (u_1, u_2, \ldots, u_{(n+k)})$ be an eigenvector of $\mathcal{L}(P_{n,k})$ with a second smallest eigenvalue λ_2. Then there exists some $\alpha \in \mathbf{Z}^+$ such that $u_i \ge 0$ $(1 \le i \le \alpha)$ and $u_i < 0$ $(\alpha+1 \le i \le n+k)$ or $u_i < 0$ $(1 \le i \le \alpha)$ and $u_i > 0$ $(\alpha+1 \le i \le n+k)$.

(Proof) If $U = (u_1, u_2, \ldots, u_{n+k})$ is the second eigenvector of $\mathcal{L}(P_{n,k})$, then $U \perp D^{1/2}\vec{1}$. Then by Lemma 1.4, $V^+(U) \ne \emptyset$ and $V^-(U) \ne \emptyset$. Since λ_2 is simple, there exists at most 2 sign graphs. Thus there exists some $\alpha \in \mathbf{Z}^+$ as given in the proposition. ■

Corollary 4.1
Let $U = (u_1, u_2, \ldots, u_{2(n+k)})$ be the first eigenvector of $\mathcal{L}(R_{n,k})$ and ϕ the automorphism of $R_{n,k}$. If $\phi(u_i) = u_{i+n+k}$ $(i = 1, \ldots, n+k)$ then $\bar{U} = (u_1, u_2, \ldots, u_{(n+k)})$ is the first eigenvector of $\mathcal{L}(P_{n,k})$.

(Proof) Let λ_1 be the first eigenvalue of $\mathcal{L}(R_{n,k})$. Then $\lambda_1 = 0$ and $U = D^{1/2}(R_{n,k})\vec{1}$. Thus $u_i = \sqrt{d_i}$ for $(i = 1, \ldots, 2(n+k))$ and the value of u_i is depend on the degree of a vertex i. Since $P_{n,k}$ and first $n+k$ vertices of $R_{n,k}$ has the same degree distribution, $D^{1/2}(R_{n,k})\vec{1} = (D^{1/2}(P_{n,k})\vec{1}, D^{1/2}(P_{n,k})\vec{1})$ and $U = (\bar{U}, \bar{U})$, where $\bar{U}$ is an eigenvector of $P_{n,k}$. Since $\bar{U} = D^{1/2}(P_{n,k})\vec{1}$, $\bar{U}$ is the first eigenvector of $\mathcal{L}(P_{n,k})$. ■

Proposition 4.5
Let $U = (u_1, u_2, \ldots, u_{2(n+k)})$ be an eigenvector of $\mathcal{L}(R_{n,k})$ with the second smallest eigenvalue λ_2. If U is an even vector then $\bar{U} = (u_1, u_2, \ldots, u_{n+k})$ is the second eigenvector of $\mathcal{L}(P_{n,k})$ with the same eigenvalue λ_2.

(Proof) Since U is an even vector, we can define an automorphism ϕ such that $\phi(u_i) = u_{i+n+k}$ for $(i = 1, \ldots, n+k)$ and U can be written as $U = (\bar{U}, \bar{U})$. Then $\bar{U}$ is an eigenvector of $\mathcal{L}(P_{n,k})$ with eigenvalue λ_2 by the Proposition 4.3. Since U is a second eigenvector of $R_{n,k}$, $U \perp D^{1/2}(R_{n,k})\vec{1}$ and $\lambda_2 > 0$. Then we have $\bar{U} \perp D^{1/2}(P_{n,k})\vec{1}$. This shows that $\bar{U}$ is an eigenvector with second smallest eigenvalue λ_2.

■

Lemma 4.1
Let $U = (u_1, \ldots, u_{2(n+k)})$ be a second eigenvector of $\mathcal{L}(R_{n,k})$. If U is an odd vector then

1. *$u_i > 0$ for $1 \le i \le n+k$ and $u_i < 0$ for $n+k+1 \le i \le 2(n+k)$ or*
2. *$u_i < 0$ for $1 \le i \le n+k$ and $u_i > 0$ for $n+k+1 \le i \le 2(n+k)$.*

(Proof) Let $V_1 = \{i \mid 1 \le i \le \alpha, u_i > 0\}$ and $V_2 = \{i \mid \alpha+1 \le i \le n+k, u_i < 0\}$, where $1 \le \alpha \le n+k$. Since U is an odd vector, there exists an automorphism ϕ such that $\phi(u_i) = -u_{(n+k+i)}$, where $1 \le i \le n+k$. Then we have $V_3 = \{i \mid n+k+1 \le i \le n+k+\alpha, \phi(u_i) < 0\}$ and $V_4 = \{i \mid n+k+\alpha+1 \le i \le 2(n+k), \phi(u_i) > 0\}$. Now for any vertex $i \in V_1 \cup V_4$, we have $u_i > 0$ and for any $i \in V_2 \cup V_3$, we have $u_i < 0$. For any $i \in V_1$ and $j \in V_4$, $(i,j) \notin E(R_{n,k})$, where $1 \le i \le \alpha$ and $n+k+\alpha+1 \le j \le 2(n+k)$. It is clear that V_1 and V_4 are disconnected sets and therefore we have two positive sign graphs V_1 and V_4. Similarly, there exists two negative sign graphs V_2 and V_3. Since the second eigenvector has no more than two sign graphs, this contradicts the nodal domain theorem [14]. Therefore eigenvector entries of vertices belongs to V_1 and V_2 should have the same sign. This implies the existence of two partitions such that $\{i \mid 1 \le i \le n+k\}$ and $\{i \mid n+k+1 \le i \le 2(n+k)\}$. Similarly, we can prove the part 2. ■

Lemma 4.2
Let $U = (u_1, \ldots, u_{2(n+k)})$ be a second eigenvector of $\mathcal{L}(R_{n,k})$. If U is an even vector then we have,

1. *$u_i > 0$ for $(1 \le i \le \alpha) \vee (n+k+1 \le i \le n+k+\alpha)$ and $u_i < 0$ for $(\alpha+1 \le i \le n+k) \vee (n+k+\alpha+1 \le i \le 2(n+k))$ or*
2. *$u_i < 0$ for $(1 \le i \le \alpha) \vee (n+k+1 \le i \le n+k+\alpha)$ and $u_i > 0$ for $(\alpha+1 \le i \le n+k) \vee (n+k+\alpha+1 \le i \le 2(n+k))$,*

where $n < \alpha < n+k$ and $\alpha \in \mathbf{Z}^+$.

(Proof) Let $V_1 = \{i \mid 1 \le i \le \alpha, u_i > 0\}$ and $V_2 = \{i \mid \alpha+1 \le i \le n+k, u_i < 0\}$, where $1 \le \alpha \le n$. Since U is an even vector, there exists an automorphism ϕ such that $\phi(u_i) = u_{(n+k+i)}$ for $1 \le i \le n+k$. Then there exist a set $V_3 = \{i \mid n+k+1 \le i \le n+k+\alpha, \phi(u_i) > 0\}$ and $V_4 = \{i \mid n+k+\alpha+1 \le i \le 2(n+k), \phi(u_i) < 0\}$. $u_i > 0$ for $i \in V_1 \cup V_3$ and $u_i < 0$ for any vertex $i \in V_2 \cup V_4$. For any $i \in V_1$ and $j \in V_3$, $(i,j) \notin E(R_{n,k})$. Therefore V_1 and V_3 are disconnected and have two positive sign graphs V_1 and V_3. Since the second eigenvector has no more than two sign graphs this contradicts the nodal domain theorem [14]. Then $\alpha > n$. For any vertex $i \in V_2$ and $j \in V_4$, $(i,j) \in E(R_{n,k})$. Hence we have one negative sign graph $V_2 \cup V_4$ and one positive sign graph $V_1 \cup V_3$. Therefore we have two sets such that $\{i \mid 1 \le i \le \alpha\} \cup \{i \mid n+k+1 \le i \le n+k+\alpha\}$ and $\{i \mid \alpha+1 \le i \le n+k\} \cup \{i \mid n+k+\alpha+1 \le i \le 2(n+k)\}$. Similarly, we can prove the part 2 of the

lemma. ■

Proposition 4.6
For the graph $R_{n,k}(n \geq 1, k > 1)$, if n and k belong to the following region R then $Mcut(R_{n,k}) < Lcut(R_{n,k})$.

$$\begin{aligned} R &= \{(n,k) \mid ((k \geq 4) \wedge (2 \mid k) \wedge (3 \mid n) \wedge (1 - \frac{1}{\sqrt{2}} - \frac{3k}{2} + \frac{3k}{\sqrt{2}} \leq n)) \vee \\ &\quad (k = 2 \wedge (n \geq 2)) \vee (k = 3 \wedge (n \geq 3))\}. \end{aligned}$$

(Proof) If n and k belong to the above region R then $Mcut(R_{n,k}) = \dfrac{(6k+4n-4)}{(2n-1)(6k+2n-3)}$ and denoted by c_2 in the Proposition 2.4. Let ϕ be an automorphism defined on $V(R_{n,k})$ such that $v_i = \phi(v_{n+k+i})$ for $1 \leq i \leq n+k$. Let $U = (u_1, u_2, \ldots, u_{2(n+k)})$ be an eigenvector corresponding to the second smallest eigenvalue of $\mathcal{L}(R_{n,k})$. Then $\phi(u_i) = u_{n+k+i}$ or $u_i = -\phi(u_{n+k+i})$ for $1 \leq i \leq n+k$.

- *If $u_i = -\phi(u_{n+k+i})$ then the second eigenvector is odd. Then there exists a bipartition such that $A = \{v_i \mid 1 \leq i \leq n+k\}$ and $V \setminus A = \{v_i \mid n+k+1 \leq i \leq 2n+2k\}$ by Lemma 4.1. This case is denoted by c_1 in the Proposition 2.4. It is clear that c_2 is smaller than c_1 for $n > 1$ by the Proposition 2.4. If n, k is in the region R then $Mcut(R_{n,k}) < Lcut(R_{n,k})$ for $n > 1$.*

- *If $u_i = \phi(u_{n+k+i})$ then the second eigenvector is even. Then there exists a bipartition such that $A = \{v_i \mid 1 \leq i \leq \alpha\} \cup \{v_i \mid n+k+1 \leq i \leq n+k+\alpha\}$ and $V \setminus A = \{v_i \mid \alpha+1 \leq i \leq n+k\} \cup \{v_i \mid n+k+\alpha+1 \leq i \leq 2(n+k)\}$, where $n+1 \leq \alpha < (n+k)$ by Lemma 4.2. Minimum normalized cut for this kind of bipartition is represented by c_4 in the Proposition 2.4. It is clear that $c_2 < c_4$ for region R by the Proposition 2.4 and hence we obtain $Mcut(R_{n,k}) < Lcut(R_{n,k})$.*

■

4.3 The lollipop graph $LP_{n,m}$

Proposition 4.7
The second smallest eigenvalue of $\mathcal{L}(LP_{n,2})$ is simple. That is multiplicity is equal to one.

(Proof) Laplacian matrix of $LP_{n,2}$ is

$$\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & & & & 0 \\ 0 & -1 & n & -1 & \cdots & \cdots & -1 \\ \vdots & & -1 & \ddots & \ddots & & \vdots \\ \vdots & & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \vdots & & -1 & n-1 & -1 \\ 0 & 0 & -1 & \cdots & \cdots & -1 & n-1 \end{pmatrix}.$$

Since $\mathcal{L}(G)$ and $L(G)D^{-1}$ has the same spectrum by the Lemma 1.2, Characteristic polynomial of $\mathcal{L}(G)$ can be obtained by $|\lambda I - L(G)D^{-1}| = 0$, where $L(G)D^{-1}$ is

$$\begin{pmatrix} 1 & -\frac{1}{2} & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 1 & -\frac{1}{n} & 0 & \cdots & \cdots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{n-1} & \cdots & \cdots & -\frac{1}{n-1} \\ 0 & 0 & -\frac{1}{n} & 1 & \ddots & & \vdots \\ \vdots & & & -\frac{1}{n-1} & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & -\frac{1}{n-1} \\ 0 & 0 & -\frac{1}{n} & -\frac{1}{n-1} & \cdots & -\frac{1}{n-1} & 1 \end{pmatrix}.$$

The determinant of $\lambda I - L(G)D^{-1}$ is,

$$\begin{pmatrix} \lambda-1 & \frac{1}{2} & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & \lambda-1 & \frac{1}{n} & 0 & \cdots & \cdots & 0 \\ 0 & \frac{1}{2} & \lambda-1 & \frac{1}{n-1} & \cdots & \cdots & \frac{1}{n-1} \\ 0 & 0 & \frac{1}{n} & \lambda-1 & \ddots & & \vdots \\ \vdots & & & \ddots\ \frac{1}{n-1} & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \frac{1}{n-1} \\ 0 & 0 & \frac{1}{n} & \frac{1}{n-1} & \cdots & \frac{1}{n-1} & \lambda-1 \end{pmatrix}.$$

For simplicity let $\lambda I - D^{-1}L(G)$ as M. By expanding through the first column we have,

$$|M| = (\lambda-1)\begin{vmatrix} \lambda-1 & \frac{1}{n} & 0 & \cdots & \cdots & 0 \\ \frac{1}{2} & \lambda-1 & \frac{1}{n-1} & \cdots & \cdots & \frac{1}{n-1} \\ 0 & \frac{1}{n} & \lambda-1 & \cdots & \cdots & \frac{1}{n-1} \\ \vdots & \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & \cdots & \vdots \\ \vdots & \vdots & \vdots & & \ddots & \vdots \\ 0 & \frac{1}{n} & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix} - 1\begin{vmatrix} \frac{1}{2} & 0 & 0 & \cdots & \cdots & \cdots 0 \\ \frac{1}{2} & \lambda-1 & \frac{1}{n-1} & & \cdots & \frac{1}{n-1} \\ 0 & \frac{1}{n} & \lambda-1 & & \cdots & \frac{1}{n-1} \\ \vdots & \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & \cdots & \frac{1}{n-1} \\ \vdots & \vdots & \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & \lambda-1 \end{vmatrix}.$$

Then,

$$|M| = (\lambda-1)M_{11} - 1.M_{21}, \tag{4.3.1}$$

where,

$$M_{11} = (\lambda-1)\begin{vmatrix} \lambda-1 & \frac{1}{n-1} & & & \frac{1}{n-1} \\ \frac{1}{n} & \lambda-1 & & & \frac{1}{n-1} \\ \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & \cdots & \frac{1}{n-1} \\ \vdots & & & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix} - \frac{1}{2}\begin{vmatrix} \frac{1}{n} & 0 & & & 0 \\ \frac{1}{n} & \lambda-1 & & & \frac{1}{n-1} \\ \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & \vdots & & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix}$$

and

$$M_{21} = \frac{1}{2}\begin{vmatrix} \lambda-1 & \frac{1}{n-1} & \cdots & \cdots & \frac{1}{n-1} \\ \frac{1}{n} & \lambda-1 & & & \frac{1}{n-1} \\ \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & \vdots & & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix}.$$

Now the Equation 4.3.1 can be rewritten as

$$(\lambda-1)^2 P - \frac{(\lambda-1)}{2n}\begin{vmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 1 & \lambda-1 & & & \frac{1}{n-1} \\ 1 & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & & & \ddots & \vdots \\ 1 & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix} - \frac{1}{2}P, \tag{4.3.2}$$

where

$$P = \begin{vmatrix} \lambda-1 & \frac{1}{n-1} & & & \frac{1}{n-1} \\ \frac{1}{n} & \lambda-1 & & & \frac{1}{n-1} \\ \frac{1}{n} & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & \vdots & & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n-1} & & & \lambda-1 \end{vmatrix}.$$

Further we can deduce this to

$$(\lambda^2 - 2\lambda + \frac{1}{2})P - \frac{(\lambda-1)}{2n}Q, \tag{4.3.3}$$

where

$$Q = \begin{vmatrix} 1 & 0 & & & 0 \\ 1 & \lambda-1 & & & \frac{1}{n-1} \\ 1 & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix}.$$

Deducing all rows from row 1 in P we get,

$$\begin{vmatrix} \lambda-1 & \frac{1}{n-1} & \cdots & \cdots & \frac{1}{n-1} \\ \frac{1}{n}-\lambda+1 & \lambda-1-\frac{1}{n-1} & \cdots & \cdots & 0 \\ \frac{1}{n}-\lambda+1 & 0 & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ \frac{1}{n}-\lambda+1 & 0 & \cdots & \cdots & \lambda-1-\frac{1}{n-1} \end{vmatrix}.$$

Adding all columns to column 1 we get

$$\begin{vmatrix} \lambda & \frac{1}{n-1} & \cdots & \cdots & \frac{1}{n-1} \\ -\frac{1}{(n-1)(n)} & \lambda-\frac{n}{n-1} & & & 0 \\ -\frac{1}{(n-1)(n)} & 0 & \lambda-\frac{n}{n-1} & & 0 \\ \vdots & & & \ddots & \vdots \\ -\frac{1}{(n-1)(n)} & 0 & \cdots & \cdots & \lambda-\frac{n}{n-1} \end{vmatrix}.$$

Now expanding the determinant through the column 2 P can be reduced to

$$(\lambda-\frac{n}{n-1})\begin{vmatrix} \lambda & \frac{1}{n-1} & \cdots & \frac{1}{n-1} \\ -\frac{1}{(n-1)(n)} & \lambda-\frac{n}{n-1} & & 0 \\ \vdots & & \ddots & \vdots \\ -\frac{1}{(n-1)(n)} & 0 & \cdots & \lambda-\frac{n}{n-1} \end{vmatrix} - \frac{1}{n-1}\begin{vmatrix} -\frac{1}{n(n-1)} & 0 & \cdots & 0 \\ -\frac{1}{(n-1)(n)} & \lambda-\frac{n}{n-1} & & 0 \\ \vdots & & \ddots & \vdots \\ -\frac{1}{(n-1)(n)} & 0 & \cdots & \lambda-\frac{n}{n-1} \end{vmatrix}.$$

This can be written as

$$r_k = \alpha r_{k-1} + \frac{1}{n(n-1)^2}\cdot\alpha^{k-1}, \tag{4.3.4}$$

where $\alpha = (\lambda - \dfrac{n}{n-1})$ *and* $k = n-1$. *Consider the recurrence relation on 4.3.4.*

$$\begin{aligned} \frac{r_k}{\alpha^k} &= \frac{r_{k-1}}{\alpha^{k-1}} + \frac{1}{n(n-1)^2\alpha}, \\ \frac{r_{k-1}}{\alpha^{k-1}} &= \frac{r_{k-2}}{\alpha^{k-2}} + \frac{1}{n(n-1)^2\alpha}, \\ &\vdots \\ \frac{r_2}{\alpha^2} &= \frac{r_1}{\alpha} + \frac{1}{n(n-1)^2\alpha} \\ \frac{r_k}{\alpha^k} &= \frac{r_1}{\alpha} + (k-1)\frac{1}{n(n-1)^2\alpha}, \end{aligned} \tag{4.3.5}$$

where

$$r_1 = \begin{vmatrix} \lambda & \frac{1}{n-1} \\ -\frac{1}{n(n-1)} & \lambda-\frac{n}{n-1} \end{vmatrix} = \lambda^2 - \frac{n}{n-1}\lambda + \frac{1}{n(n-1)^2}.$$

Now P can be written as

$$P = (\lambda - \frac{n}{n-1})^{n-2}(\lambda^2 - \frac{n}{n-1}\lambda + \frac{1}{n(n-1)}). \tag{4.3.6}$$

Expanding the Q in the Equation 4.3.3 through row 1, we can write,

$$Q = \begin{vmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 1 & \lambda-1 & & & \frac{1}{n-1} \\ 1 & \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & & & \ddots & \vdots \\ 1 & \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix} = 1. \begin{vmatrix} \lambda-1 & \cdots & \cdots & \frac{1}{n-1} \\ \frac{1}{n-1} & \lambda-1 & \cdots & \frac{1}{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix}.$$

Then adding rows to the first row

$$Q = (\lambda - 1 + \frac{n-2}{n-1}) \begin{vmatrix} 1 & \cdots & \cdots & 1 \\ \frac{1}{n-1} & \lambda-1 & & \frac{1}{n-1} \\ \vdots & & \lambda-1 & \frac{1}{n-1} \\ \vdots & & \ddots & \vdots \\ \frac{1}{n-1} & \cdots & \cdots & \lambda-1 \end{vmatrix}$$

Deducing all columns from the first column becomes

$$Q = (\lambda - 1 + \frac{n-2}{n-1}) \begin{vmatrix} 1 & 0 & \cdots & 0 \\ \frac{1}{n-1} & \lambda - 1 - \frac{1}{n-1} & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ \frac{1}{n-1} & 0 & & \lambda - 1 \frac{1}{n-1} \end{vmatrix}.$$

This can be written as

$$Q = (\lambda - \frac{1}{n-1})(\lambda - \frac{n}{n-1})^{n-2}. \tag{4.3.7}$$

Substituting Equation 4.3.6 and 4.3.7 into the Equation 4.3.3 gives

$$|\lambda I - L(G)D^{-1}| = \frac{1}{2}(\lambda - \frac{n}{n-1})^{n-2} \left((2\lambda^2 - 4\lambda + 1)(\lambda^2 - \frac{n}{n-1}\lambda + \frac{1}{n(n-1)}) - \frac{\lambda - 1}{n}(\lambda - \frac{1}{n-1}) \right) \tag{4.3.8}$$

$$= \frac{1}{2n(n-1)}(\lambda - \frac{n}{n-1})^{n-2}\lambda(2n(n-1)\lambda^3 - 2n(3n-2)\lambda^2 + (5n^2 - 2n + 3)\lambda \tag{4.3.9}$$

$$+ n - n^2 - 4).$$

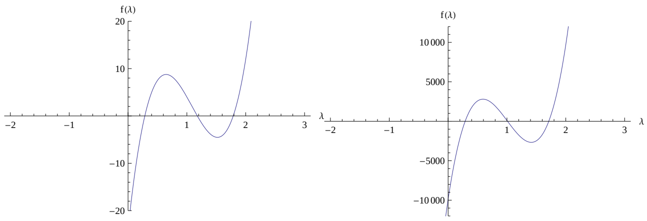
According to the Equation 4.3.9, eigenvalues of $LP_{n,2}$ is $\lambda = 0, \lambda = \dfrac{n}{n-1}$ with multiplicity $(n-2)$ and the remaining eigenvalues are the solution of the equation $2n(n-1)\lambda^3 - 2n(3n-2)\lambda^2 + (5n^2 - 2n + 3)\lambda + n - n^2 - 4 = 0$. Let

$$f(\lambda) \quad = \quad 2n(n-1)\lambda^3 - 2n(3n-2)\lambda^2 + (5n^2 - 2n + 3)\lambda + n - n^2 - 4.$$

$f(0) = -(n^2 - n + 4) < 0$ *and* $f(1) = n - 1 > 0$ *if* $n \geq 2$. $f(\frac{n}{n-1}) = -\frac{2(n-2)}{n-1} < 0$, *if* $n > 2$. $f(2) = (n-1)(n-2) > 0$ *if* $n > 2$. *This shows that there exists a solution for each interval* $0 < \lambda < 1$, $1 < \lambda < \frac{n}{n-1}$, *and* $\frac{n}{n-1} < \lambda < 2$. *Considering the graph of* $f(\lambda)$ *as in the Figure 17, it is also clear that 3 distinct roots exist and the smallest root is less than 1.* ■

Proposition 4.8
Let λ_2 *be the second smallest eigenvalue of* $\mathcal{L}(LP_{n,2})$. *If* $n \geq 5$ *then* $\lambda_2 < 1 - \frac{1}{\sqrt{2}}$ and *if* $n \leq 4$ *then* $\lambda_2 > 1 - \frac{1}{\sqrt{2}}$.

(Proof) By the Proposition 4.7, we have $0 < \lambda_2 < 1$. *Considering the equation for* $f(\lambda)$ *in the Proposition 4.7, we have* $f(1 - \frac{1}{\sqrt{2}}) = \frac{n-3-\sqrt{2}}{\sqrt{2}}$, *which is positive for* $n \geq 5$, *and negative for* $n \leq 4$. ■



(a) $m = 2, n = 5$ (b) $m = 2, n = 100$

Figure 17: Plot of $f(\lambda)$ vs λ for $n = 5$ and $n = 100$.

Proposition 4.9
Let U *be the second eigenvector of* $(LP_{n,m})$. *Then* $V^+(U) \neq \emptyset$ and $V^-(U) \neq \emptyset$.

Proof follows by the Lemma 1.4. ■

Proposition 4.10
Let λ_2 *be the second eigenvalue and* $U = (u_1, \ldots, u_{n+2})$ *the second eigenvector of* $\mathcal{L}(LP_{n,2})$. *Then*

1. $\lambda_2 \neq \frac{n}{n-1}$ and $\lambda_2 \neq \frac{1}{n-1}$.
2. $u_i = u_{i+1}$ *for* $(i = 4, \ldots, n+1)$.
3. *If* $n \geq 5$ *then* $\lambda_2 < \frac{1}{2}(2 - \sqrt{2})$ and $u_1 u_2 > 0$ and $u_1 u_3 > 0$. *That is* u_1, u_2, u_3 *are all positive or they are all negative values.*

4. If $n \geq 5$ then u_1, u_2, u_3 are positive and $u_i (i = 4, \ldots, n+2)$ are negative or u_1, u_2, u_3 are negative and $u_i (i = 4, \ldots, n+2)$ are positive. That is u_3 and u_4 have opposite signs.

5. If $n = 3$ or $n = 4$ then $\lambda_2 > \frac{1}{2}(2 - \sqrt{2})$ and $u_1 u_2 > 0$ and $u_1 u_3 < 0$. That is if u_1, u_2 are positive then u_3 is negative or if u_1, u_2 are negative then u_3 is positive.

6. If $n = 3, 4$ then u_1, u_2 are positive and $u_i (i = 3, \ldots, n+2)$ are negative or vice versa.

(Proof)

1. From the Proposition 4.7, $f(\lambda) = 2n(n-1)\lambda^3 - 2n(3n-2)\lambda^2 + \left(5n^2 - 2n + 3\right)\lambda + n - n^2 - 4$. If $\lambda = \dfrac{1}{n-1}$ then $f(\lambda) = -7 + 6n - n^2 \neq 0$ and if $\lambda = \dfrac{n}{n-1}$ then $-\dfrac{2(-2+n)}{-1+n} \neq 0$.

2. According to the vertex numbering of $LP_{n,2}$ the normalized Laplacian matrix of $LP_{n,2}$ is,

$$\begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{\sqrt{2n}} & \cdots & & 0 \\ 0 & -\frac{1}{\sqrt{2n}} & 1 & & & -\frac{1}{\sqrt{n(n-1)}} \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & 1 & -\frac{1}{n-1} \\ 0 & \cdots & \cdots & \cdots & -\frac{1}{n-1} & 1 \end{pmatrix}.$$

Since $\mathcal{L}(LP_{n,2})U = \lambda_2 U$, we have the following system of equations.

$$-\frac{1}{\sqrt{2}} u_2 + u_1 = \lambda_2 u_1, \tag{4.3.10}$$

$$-\frac{1}{\sqrt{2n}} u_3 + u_2 - \frac{1}{\sqrt{2}} u_1 = \lambda_2 u_2, \tag{4.3.11}$$

$$-\frac{1}{\sqrt{n(n-1)}} (u_{n+2} + \cdots + u_4) + u_3 - \frac{1}{\sqrt{2n}} u_2 = \lambda_2 u_3, \tag{4.3.12}$$

$$-\frac{1}{\sqrt{n(n-1)}} u_3 - \frac{1}{n-1} (u_{n+2} + \cdots + u_5) + u_4 = \lambda_2 u_4, \tag{4.3.13}$$

$$-\frac{1}{\sqrt{n(n-1)}} u_3 - \frac{1}{n-1} (u_4 + \cdots + u_{n+2}) + u_5 = \lambda_2 u_5, \tag{4.3.14}$$

$$\vdots \tag{4.3.15}$$

$$-\frac{1}{\sqrt{n(n-1)}} u_3 - \frac{1}{n-1} (u_4 + \cdots + u_{n+1}) + u_{n+2} = \lambda_2 u_{n+2}. \tag{4.3.16}$$

By solving the system of equations from the Equation 4.3.13 to Equation 4.3.16, we have $u_4 = u_5 = \cdots = u_{n+2}$. That is $u_i = u_{i+1}$ for $i = 4, \ldots, n+1$.

3. *By simplifying the Equation 4.3.10,Equation 4.3.11 and the Equation 4.3.12, we have*

$$\begin{aligned} u_2 &= \sqrt{2}(1-\lambda_2)u_1, \\ u_3 &= \sqrt{n}(2(1-\lambda_2)^2-1)u_1, \\ \sqrt{\frac{n-1}{n}}u_4 &= (1-\lambda_2)u_3 - \frac{1}{\sqrt{2n}}u_2. \end{aligned}$$

   If $u_1 > 0$ then $u_2 > 0$ and this implies that $u_1u_2 > 0$. If $u_1 < 0$ then $u_2 < 0$ and this also implies that $u_1u_2 > 0$. If $u_1 > 0$ then $u_3 > 0$, whenever $2(1-\lambda_2)^2 - 1 > 0$. That is $(\lambda_2 - \frac{(2-\sqrt{2})}{2})(\lambda_2 - \frac{(2+\sqrt{2})}{2}) > 0$. It is clear that $(\lambda_2 - \frac{(2+\sqrt{2})}{2}) < 0$ since $\lambda_2 < 1$. For $n \geq 5$, $\lambda_2 < \frac{(2-\sqrt{2})}{2}$ by the Proposition 4.8. Hence $u_3 > 0$ whenever $u_1 > 0$ for $n \geq 5$. Similarly, if $u_1 < 0$ then $u_3 < 0$ for $n \geq 5$. That is u_1, u_2, u_3 are all positive or all negative.

4. *Since U is the second eigenvector, $U \perp D^{1/2}\vec{1}$ and $\sum_{i=1}^{n+2} u_i.\sqrt{d_i} = 0$. Since $d_4 = \cdots = d_{n+2} = n-1$, we have, $u_1 + \sqrt{2}u_2 + \sqrt{n}u_3 + (n-1)\sqrt{n-1}u_4 = 0$. This implies that if $u_1, u_2, u_3 > 0$ then $u_4, \ldots, u_{n+2} < 0$ and if $u_1, u_2, u_3 < 0$ then $u_4, \ldots, u_{n+2} > 0$.*

5. *By the Equation 4.3.10, if $u_1 > 0$ then $u_2 > 0$ and $u_1u_2 > 0$. If $u_1 < 0$ then $u_2 < 0$ and again $u_1u_2 > 0$. If $n = 3$ or $n = 4$ then $\lambda_2 > (1 - \frac{1}{\sqrt{2}})$ by the Proposition 4.8. That is if $u_1 > 0$ then $u_3 < 0$ from the Equation 4.3.11.*

6. *From the part(1), we have $u_i = u_{i+1}(i = 4, \ldots, n+1)$. If $n = 3, 4$ and $u_1, u_2 > 0$ then $u_3 < 0$ from the part (5). If $u_i(i = 4, \ldots, n+2) > 0$ then we have 3 connected sign graphs which contradicts the nodal domain theorem [14]. Hence we have $u_i(i = 4, \ldots, n+2) < 0$. That is if $u_3 < 0$ then $u_i(i = 4, \ldots, n+2) < 0$ or if $u_3 > 0$ then $u_i(i = 4, \ldots, n+2) > 0$. This implies that if u_1, u_2 have a same sign then $u_i(i = 3, \ldots, n+2)$ have a opposite sign.*

■

Corollary 4.2
Let $U = (u_1, \ldots, u_{n+2})$ be the second eigenvector of $\mathcal{L}(LP_{n,2})$. Then for $n \geq 5$, $u_i > 0, (4 \leq i \leq n+2)$ and $u_i < 0 (i \leq 3)$ or $u_i < 0 (4 \leq i \leq n+2)$ and $u_i > 0 (i \leq 3)$ and the graph $LP_{n,2}$ can partition by cutting edges between vertex y_1 and vertices $y_2, \ldots, y_n$.

(Proof) Proofs follows by the Proposition 4.10. That is if $n \geq 5$ and u_1, u_2, u_3 are positive then $u_i(i = 4, \ldots, n+2)$ are negative. Hence graph can be separated by cutting all edges between vertex y_1 and $y_2, \ldots, y_n$. ■

Proposition 4.11
$Mcut(LP_{n,m}) < Lcut(LP_{n,m})$ for $n \geq 5$ and $m = 2$.

(Proof) For $m = 2$ we have, $Mcut(LP_{n,2}) = \frac{n^2-n+4}{3(n^2-n+1)}$ by the Proposition 2.6. For $n \geq 5$, there exists a subset $A \subset V(LP_{n,2})$ such that $A = \{x_1, x_2, y_1\}$ and $V \setminus A = \{y_i \mid 2 \leq i \leq n+2\}$

by the Corollary 4.2. Then $cut(A, V \setminus A) = n - 1$, $vol(A) = n + 3$ and $vol(V \setminus A) = (n-1)^2$. Thus $Lcut(LP_{n,2}) = (n-1)\left(\frac{1}{n+3} + \frac{1}{(n-1)^2}\right) = \frac{n^2 - n + 4}{(n-1)(n+3)}$. Comparing $Mcut(LP_{n,2})$ with $Lcut(LP_{n,2})$, we have $Mcut(LP_{n,2}) < Lcut(LP_{n,2})$. ■

We proved that $Mcut(LP_{n,m}) \neq Lcut(LP_{n,m})$ for $n \geq 5, m = 2$. There are some other cases, which we can prove similar to the previous Proposition 4.11. We list some of them in the following conjecture.

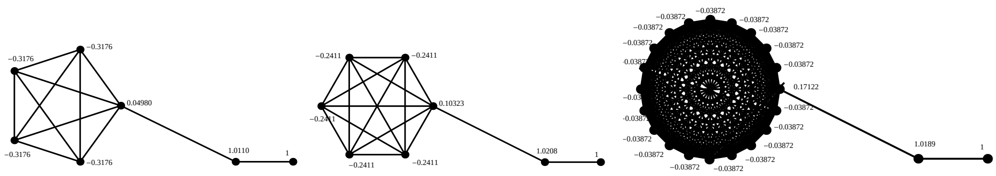
Conjecture 4.1
For the graph $LP_{n,m}$, $Lcut(LP_{n,m}) \neq Mcut(LP_{n,m})$, when $n > m$ and the following conditions hold.

1. $m = 3, n \geq 9$,
2. $m = 4, n \geq 15$, and
3. $m = 5, n \geq 22$.

Similarly, $Lcut(LP_{n,m}) \neq Mcut(LP_{n,m})$, when $m > n$ and the following conditions hold:

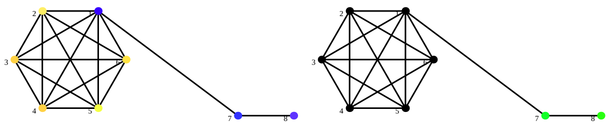
1. $m = 7, 3 \leq n \leq 5$,
2. $m = 10, 3 \leq n \leq 9$,
3. $m = 19, 3 \leq n \leq 15$, and
4. $m = 27, 3 \leq n \leq 22$.

Example 4.3
The Figure 18 shows the second eigenvector of $\mathcal{L}(LP_{n,2})$ for $n = 5, 6, 20$. The Figure 19 shows the bipartition enumerated by $Mcut(LP_{6,2})$ and $Lcut(LP_{6,2})$.



(a) $m = 2, n = 5$ (b) $m = 2, n = 6$ (c) $m = 2, n = 20$

Figure 18: Second smallest eigenvector of $LP_{n,m}$.



(a) $Lcut$ for $LP_{6,2}$ (b) $Mcut$ of $LP_{6,2}$

Figure 19: $Lcut$ and $Mcut$ of $LP_{6,2}$.

4.4 The graph $LP'_{n,2}$

Proposition 4.12

Let λ_2 be the second smallest eigenvalue and $U = (u_1, u_2, \dots, u_{n+2})$ be the second eigenvector of $LP'_{n,2}$. Then the following conditions hold.

1. *$u_i = u_{i+1}$ for $(i = 4, \dots, n)$.*
2. *$u_1 = u_2$ and $u_3 = u_{n+2}$.*
3. *For $n \geq 6$, $\lambda_2 < \dfrac{1}{2}$.*
4. *For $n \geq 6$, $u_2 u_3 > 0$. That is u_1, u_2, u_3, u_4 are all positive numbers or they are all negative numbers.*
5. *For $n = 5$, $u_2 u_3 = 0$. That is u_1, u_2 are all positive numbers or they are all negative numbers and u_2, u_3 are zeros.*

(Proof)

1. *Normalized Laplacian of $LP'_{n,2}$ can be written as,*

$$\begin{pmatrix}
1 & -\frac{1}{2} & 0 & \cdots & \cdots & -\frac{1}{\sqrt{2n}} \\
-\frac{1}{2} & 1 & -\frac{1}{\sqrt{2n}} & \cdots & \cdots & 0 \\
0 & -\frac{1}{\sqrt{2n}} & 1 & \ddots & & -\frac{1}{n} \\
\vdots & & \ddots & \ddots & \ddots & \vdots \\
\vdots & & & & 1 & -\frac{1}{\sqrt{n(n-1)}} \\
-\frac{1}{\sqrt{2n}} & 0 & -\frac{1}{n} & \cdots & -\frac{1}{\sqrt{n(n-1)}} & 1
\end{pmatrix}.$$

Then $\lambda_2 U - \mathcal{L}(LP'_{n,2})U = 0$. *Considering the first 3 rows of* $\mathcal{L}(LP'_{n,2})$,

$$(\lambda_2 - 1)u_1 + \frac{1}{2}u_2 + \frac{1}{\sqrt{2n}}u_{n+2} = 0, \quad (4.4.1)$$

$$\frac{1}{\sqrt{2n}}u_3 + (\lambda_2 - 1)u_2 + \frac{1}{2}u_1 = 0, \quad (4.4.2)$$

$$\frac{1}{\sqrt{n(n+1)}}(u_{n+1} + \cdots + u_4) + (\lambda_2 - 1)u_3 + \frac{1}{\sqrt{2n}}u_2 + \frac{1}{n}u_{n+2} = 0. \quad (4.4.3)$$

Since $LP'_{n,2} \setminus \{u_1, u_2\}$ *is a complete graph, we can write* $n-1$ *equations as follows.*

$$\frac{1}{(n-1)}(u_{n+1} + \cdots + u_5) + (\lambda_2 - 1)u_4 + \frac{1}{\sqrt{n(n-1)}}u_3 + \frac{1}{\sqrt{n(n-1)}}u_{n+2} = 0, \quad (4.4.4)$$

$$\frac{1}{(n-1)}(u_{n+1} + \cdots + u_6 + u_4) + (\lambda_2 - 1)u_5 + \frac{1}{\sqrt{n(n-1)}}u_3 + \frac{1}{\sqrt{n(n-1)}}u_{n+2} = 0, \quad (4.4.5)$$

$$\vdots$$

$$\frac{1}{\sqrt{n(n-1)}}(u_4 + \cdots + u_{n+1}) + \frac{1}{n}u_3 + \frac{1}{\sqrt{2n}}u_1 + (\lambda_2 - 1)u_{n+2} = 0. \quad (4.4.6)$$

By solving the Equation 4.4.4, and the Equation 4.4.5 we have, $u_4 = u_5$. *Similarly, we can obtain,* $u_4 = u_5 = \cdots = u_{n+1}$ *by solving system of equations from Equation 4.4.4 to Equation 4.4.6.*

2. *From the Equation 4.4.1, 4.4.2,*

$$\begin{aligned} u_2 &= 2(1-\lambda_2)u_1 - 2\frac{1}{\sqrt{2n}}u_{n+2}, \\ u_3 &= \sqrt{2n}((1-\lambda_2)u_2 - \frac{1}{2}u_1). \end{aligned}$$

From the Equation 4.4.3, 4.4.5 we have

$$\frac{n-2}{\sqrt{n(n-1)}}u_4 + (\lambda_2 - 1)u_3 + \frac{1}{\sqrt{2n}}u_2 + \frac{1}{n}u_{n+2} = 0, \quad (4.4.7)$$

$$\frac{n-2}{\sqrt{n(n-1)}}u_4 + \frac{1}{n}u_3 + \frac{1}{\sqrt{2n}}u_1 + (\lambda_2 - 1)u_{n+2} = 0. \quad (4.4.8)$$

Solving the Equation 4.4.1 and 4.4.2, we have,

$$\frac{1}{\sqrt{2n}}(u_{n+2} - u_3) = (\frac{3}{2} - \lambda_2)(u_1 - u_2). \quad (4.4.9)$$

By solving the Equation 4.4.7 and 4.4.8 we have,

$$(\frac{1}{n} - \lambda_2 + 1)(u_{n+2} - u_3) = \frac{1}{\sqrt{2n}}(u_1 - u_2). \quad (4.4.10)$$

By solving the Equation 4.4.9 and 4.4.10, we get the solution $u_{n+2} = u_3$ *and* $u_1 = u_2$.

3. If $n = 3$ then $\lambda_2 \leq Mcut(LP'_{3,2}) = 0.75$ and $\lambda_2 = 2/3$ by computations. If $n = 4$ then $\lambda_2 \leq 9/14 = 0.6428$ and $\lambda_2 = 0.54$. If $n = 5$ then $\lambda_2 \leq 13/22 = 0.59$ and $\lambda_2 = 0.5$. If $n \geq 6$ then $\lambda_2 < 0.5$.

4. Let $n \geq 6$. If $u_1 > 0$ then $u_2 > 0$. Let $u_1 > 0$. Then $u_3 = u_{n+2} > 0$ or $u_3 = u_{n+2} < 0$. If $u_3 = u_{n+2} > 0$ then $u_4 = u_5 = \cdots = u_{n+1} < 0$. Otherwise it contradicts that the second eigenvector is orthogonal to $D^{1/2}\vec{1}$. If $u_3 = u_{n+2} < 0$ and $u_4 = u_5 = \cdots = u_{n+1} > 0$, then we have 3 sign graphs and contradicts the nodal domain theorem [14]. Therefore $u_4 = u_5 = \cdots = u_{n+1} < 0$. From the Equation 4.4.1, $(\lambda_2 - \frac{1}{2})u_1 = -\frac{1}{\sqrt{2n}}u_{n+2}$. Therefore if $u_1 > 0$ then $u_{n+2} > 0$. Similarly when $u_1 < 0$ we have $u_{n+2} = u_3 < 0$. That is u_1, u_2, u_3, u_{n+2} have the same sign.

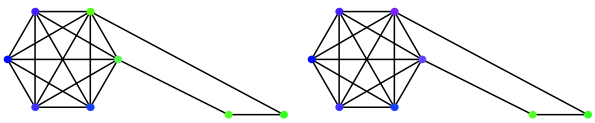
5. If $n = 5$ then $\lambda_2 = 0.5$. So we have $u_{n+2} = u_3 = 0$. If $u_1 > 0$ then $u_2 > 0$. Then we have $u_i (i = 4, \ldots, n+1) < 0$. If $u_1 < 0$ then $u_2 < 0$ and we have $u_i(i = 4, \ldots, n+1) > 0$. That is $u_1 u_3 = 0$.

■

Proposition 4.13
$Lcut(LP'_{n,2}) < Mcut(LP'_{n,2})$ for $n \geq 5$.

(Proof) If $n \geq 5$ then $\lambda_2 \leq 0.5$ and the second eigenvector separate the graph into two groups such that u_1, u_2, u_3, u_{n+2} belong to one group and $u_4, \ldots, u_{n+1}$ belong to other group by the Proposition 4.12. Then $Lcut(LP'_{n,2}) = \frac{n^2 - n + 6}{(n+2)(n-1)}$ by the Proposition 2.7. But $Mcut(LP'_{n,2}) = \frac{n^2 - n + 6}{2(n^2 - n + 2)}$ by the Proposition 2.7. Comparing $Lcut$ and $Mcut$ values, we have $Lcut(LP'_{n,2}) < Mcut(LP'_{n,2})$ for $n \geq 5$.
■

Example 4.4
The Figure 20 shows the bipartition produced by $Lcut(LP'_{n,2})$ and $Mcut(LP'_{n,2})$ for $n = 6$.



(a) $Lcut$ for $LP'_{6,2}$ (b) $Mcut$ of $LP'_{6,2}$

Figure 20: $Lcut$ and $Mcut$ of $LP'_{6,2}$.

4.5 Double tree

In this section, we show that the second eigenvector of double tree is odd and $Lcut(DT_n) = Mcut(DT_n)$ *for any* $n \in \mathbf{Z}^+$.

Note. *From the Proposition 2.3, we have,* $\lambda_2(DT_2) \le Mcut(DT_2) = \frac{2}{5}$. $\lambda_2(DT_3) \le Mcut(DT_3) = \frac{2}{13}$. $\lambda_2(DT_n) \le Mcut(DT_n) = \frac{2}{2^{n+1}-3} < 1$. ■

Proposition 4.14
Let λ_2 *be the second smallest eigenvalue of* $\mathcal{L}(DT_n)$ *and* $U = (U_i), i \in V(DT_n)$ *be the second smallest eigenvector of* $\mathcal{L}(DT_n)$. *Then the following relations hold for* $w \in \Sigma^{\le n}$.

1. *If there exists* $x(w) \in V(DT_n)$ *such that* $U_{x(w)} > 0$ *then* $U_{x(w)} > 0$ *for all* $w \in \Sigma^{\le n}$.
2. *If there exists* $x(w) \in V(DT_n)$ *such that* $U_{x(w)} > 0$ *then* $U_{y(w)} < 0$.

(Proof) Let $n = 2$ *and* $w \in \Sigma^{\le n}, |wu| = |w| + 1$ *and* $u \in \{0, 1\}$. *Then*

$$\mathcal{L}(DT_2) = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix},$$

where $A = (a_{x(w),x(wu)})$ *is the matrix defined as*

$$\begin{cases} 1 & \text{if } x(w) = x(wu), \\ -\frac{1}{\sqrt{d_{x(w)}d_{x(wu)}}} & \text{if } (x(w), x(wu)) \in E(DT_2), \\ 0 & \text{otherwise,} \end{cases}$$

$B = (b_{y(w),y(wu)})$ *is the matrix defined as*

$$\begin{cases} 1 & \text{if } y(w) = y(wu), \\ -\frac{1}{\sqrt{d_{y(w)}d_{y(uw)}}} & \text{if } (y(w), y(wu)) \in E(DT_2), \\ 0 & \text{otherwise,} \end{cases}$$

$C = (c_{x(w),y(w)})$ *is the matrix defined as*

$$\begin{cases} -\frac{1}{\sqrt{d_{x(w)}d_{y(w)}}} & \text{if } w = \epsilon, \\ 0 & \text{otherwise.} \end{cases}$$

Let U *be the second eigenvector such that*

$$U = \begin{pmatrix} U_{x(w)} \\ U_{y(w)} \end{pmatrix},$$

where $U_{x(w)} = (U_{x(\epsilon)}, U_{x(0)}, U_{x(1)})$ *and* $U_{y(w)} = (U_{y(\epsilon)}, U_{y(0)}, U_{y(1)})$. *Each vertex of the bottom level has degree 1 and vertices of the other levels has degree 3. Hence for simplicity, let* α *as* $d_{x(w)}$, *where for* $w \in \Sigma^{\le n}$ *and* $|w| \le n - 2$. *All other vertices* $x(w)$ *such that* $|w| = n - 1$ *has* $d(x(w)) = 1$. *Since* DT_2 *has a symmetric structure,* $A = B$. *Then we can write the following equations.*

$$\begin{aligned} AU_{x(w)} + CU_{y(w)} &= \lambda_2 U_{x(w)}, \\ C^T U_{x(w)} + AU_{y(w)} &= \lambda_2 U_{y(w)}. \end{aligned}$$

Then

$$A = \begin{pmatrix} 1 & -\frac{1}{\sqrt{\alpha}} & -\frac{1}{\sqrt{\alpha}} \\ -\frac{1}{\sqrt{\alpha}} & 1 & 0 \\ -\frac{1}{\sqrt{\alpha}} & 0 & 1 \end{pmatrix},$$

$$C = \begin{pmatrix} -\frac{1}{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$U_{x(w)} = \begin{pmatrix} U_{x(\epsilon)} \\ U_{x(0)} \\ U_{x(1)} \end{pmatrix},$$

and

$$U_{y(w)} = \begin{pmatrix} U_{y(\epsilon)} \\ U_{y(0)} \\ U_{y(1)} \end{pmatrix}.$$

$AU_{x(w)} + CU_{y(w)} = \lambda_2 U_{x(w)}$ *implies that,*

$$U_{x(\epsilon)} - \frac{1}{\sqrt{\alpha}}U_{x(0)} - \frac{1}{\sqrt{\alpha}}U_{x(1)} - \frac{1}{\alpha}U_{y(\epsilon)} = \lambda_2 U_{x(\epsilon)}, \tag{4.5.1}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(\epsilon)} + U_{x(0)} = \lambda_2 U_{x(0)}, \tag{4.5.2}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(\epsilon)} + U_{x(1)} = \lambda_2 U_{x(1)}. \tag{4.5.3}$$

$C^T U_{x(w)} + AU_{y(w)} = \lambda_2 U_{y(w)}$ *implies that,*

$$U_{y(\epsilon)} - \frac{1}{\sqrt{\alpha}}U_{y(0)} - \frac{1}{\sqrt{\alpha}}U_{y(1)} - \frac{1}{\alpha}U_{x(\epsilon)} = \lambda_2 U_{y(\epsilon)}, \tag{4.5.4}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(\epsilon)} + U_{y(0)} = \lambda_2 U_{y(0)}, \tag{4.5.5}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(\epsilon)} + U_{y(1)} = \lambda_2 U_{y(1)}. \tag{4.5.6}$$

From the Equation 4.5.1, 4.5.2, 4.5.3,

$$U_{x(0)} = U_{x(1)}, \tag{4.5.7}$$

$$U_{x(\epsilon)} - \frac{2}{\sqrt{\alpha}}U_{x(1)} - \frac{1}{\alpha}U_{y(\epsilon)} = \lambda_2 U_{x(\epsilon)}. \tag{4.5.8}$$

From the Equation 4.5.4, 4.5.5, 4.5.6,

$$U_{y(0)} = U_{y(1)}, \tag{4.5.9}$$

$$U_{y(\epsilon)} - \frac{2}{\sqrt{\alpha}}U_{y(1)} - \frac{1}{\alpha}U_{x(\epsilon)} = \lambda_2 U_{y(\epsilon)}. \tag{4.5.10}$$

Then by solving the Equation 4.5.2, 4.5.8 and 4.5.5, 4.5.10, $U^2_{x(\epsilon)} = U^2_{y(\epsilon)}$. *This implies that* $U_{x(\epsilon)} = U_{y(\epsilon)}$ *or* $U_{x(\epsilon)} = -U_{y(\epsilon)}$. *Above equations have non zero solutions for* $U_{x(\epsilon)}, \ldots, U_{x(1)}, U_{y(\epsilon)}, \ldots, U_{y(1)}$ *if* $\lambda_2 \neq 1$. *But* $\lambda_2 \leq Mcut(G) = \frac{2}{5}$ *from the Proposition 4.5. If* $U_{x(\epsilon)} = U_{y(\epsilon)}$ *then by the Equation 4.5.5, 4.5.2* $U_{x(0)} = U_{y(0)}$ *and by the Equation 4.5.3, 4.5.6* $U_{x(1)} = U_{y(1)}$. *If* $U_{x(\epsilon)} > 0$ *then from the Equation 4.5.2,* $U_{x(0)} > 0$ *and hence* $U_{x(1)} > 0$.

If we take $U_{x(\epsilon)} = U_{y(\epsilon)}$ *then* $U_{x(\epsilon)}, U_{x(0)}, U_{x(1)}, U_{y(\epsilon)}, U_{y(0)}$ *and* $U_{y(1)}$ *have same sign. It contradicts that second eigenvector is orthogonal to* $D^{1/2}\vec{1}$. *So we can exclude this case and consider the case* $U_{x(\epsilon)} = -U_{y(\epsilon)}$. *This implies that* $U_{x(w)} > 0$ *and* $U_{y(w)} < 0$ *for all* $w \in \Sigma^{\leq n}$. *Hence the eigenvector for* U *is* $U_{x(\epsilon)}, U_{x(0)}, U_{x(1)}, -U_{x(\epsilon)}, -U_{x(0)}, -U_{x(1)}$. *This implies that if* $U_{x(w)} > 0$ *then for all* $x(w), U_{x(w)} > 0$ *and if* $U_{x(w)} > 0$ *then for all* $y(w)$, $U_{y(w)} < 0$. *Hence the second eigenvector is odd and partition the graph by cutting an edge between their roots.*

Now let $n = 3$ *and consider the graph* DT_3. *Similar to the previous proof, we have the following system of equations.*

$$U_{x(\epsilon)} - \frac{1}{\alpha}U_{x(0)} - \frac{1}{\alpha}U_{x(1)} - \frac{1}{\alpha}U_{y(\epsilon)} = \lambda_2 U_{x(\epsilon)}, \tag{4.5.11}$$

$$-\frac{1}{\alpha}U_{x(\epsilon)} + U_{x(0)} - \frac{1}{\sqrt{\alpha}}U_{x(00)} - \frac{1}{\sqrt{\alpha}}U_{x(01)} = \lambda_2 U_{x(0)}, \tag{4.5.12}$$

$$-\frac{1}{\alpha}U_{x(\epsilon)} + U_{x(1)} - \frac{1}{\sqrt{\alpha}}U_{x(10)} - \frac{1}{\sqrt{\alpha}}U_{x(11)} = \lambda_2 U_{x(1)}, \tag{4.5.13}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(0)} + U_{x(00)} = \lambda_2 U_{x(00)}, \tag{4.5.14}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(0)} + U_{x(01)} = \lambda_2 U_{x(01)}, \tag{4.5.15}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(1)} + U_{x(10)} = \lambda_2 U_{x(10)}, \tag{4.5.16}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(1)} + U_{x(11)} = \lambda_2 U_{x(11)}, \tag{4.5.17}$$

$$U_{y(\epsilon)} - \frac{1}{\alpha}U_{y(0)} - \frac{1}{\alpha}U_{y(1)} - \frac{1}{\alpha}U_{x(\epsilon)} = \lambda_2 U_{y(\epsilon)}, \tag{4.5.18}$$

$$-\frac{1}{\alpha}U_{y(\epsilon)} + U_{y(0)} - \frac{1}{\sqrt{\alpha}}U_{y(00)} - \frac{1}{\sqrt{\alpha}}U_{y(01)} = \lambda_2 U_{y(0)}, \tag{4.5.19}$$

$$-\frac{1}{\alpha}U_{y(\epsilon)} + U_{y(1)} - \frac{1}{\sqrt{\alpha}}U_{y(10)} - \frac{1}{\sqrt{\alpha}}U_{y(11)} = \lambda_2 U_{y(1)}, \tag{4.5.20}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(0)} + U_{y(00)} = \lambda_2 U_{y(00)}, \tag{4.5.21}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(0)} + U_{y(01)} = \lambda_2 U_{y(01)}, \tag{4.5.22}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(1)} + U_{y(10)} = \lambda_2 U_{y(10)}, \tag{4.5.23}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(1)} + U_{y(11)} = \lambda_2 U_{y(11)}. \tag{4.5.24}$$

$U_{x(00)} = U_{x(01)}, U_{x(10)} = U_{x(11)}$ *by the Equation 4.5.14, 4.5.15 and 4.5.16, 4.5.17. Similarly* $U_{y(00)} = U_{y(01)}, U_{y(10)} = U_{y(11)}$ *by the Equation 4.5.21, 4.5.22 and 4.5.23, 4.5.24. By solving the equation set 4.5.12, 4.5.13, 4.5.14, 4.5.16 with the condition* $U_{x(00)} = U_{x(01)}$ *and* $U_{x(10)} = U_{x(11)}$*, we have* $U_{x(0)} = U_{x(1)}$*. Similarly we can obtained the result* $U_{y(0)} = U_{y(1)}$*. By solving the Equation 4.5.11, 4.5.14, 4.5.16 and the Equation 4.5.19, 4.5.21 we have* $U^2_{x(\epsilon)} = U^2_{y(\epsilon)}$*. If* $U_{y(\epsilon)} = U_{x(\epsilon)}$ *then all vectors are positive and contradicts that the second eigenvector is orthogonal to* $D^{1/2}\vec{1}$*. Therefore* $U_{x(\epsilon)} = -U_{y(\epsilon)}$*. Since* $\lambda < \dfrac{2}{13}$*, if* $U_{x(\epsilon)} > 0$ *then* $U_{x(w)} > 0$ *for all* $w \in \Sigma_1^{\leq n}$*. Similarly, if* $U_{y(\epsilon)} < 0$ *then* $U_{y(w)} < 0$ *for all* $w \in \Sigma_1^{\leq n}$*. That is if* $U_{x(w)} > 0$ *then for all* $x(w)$*,* $U_{x(w)} > 0$ *and if* $U_{y(w)} > 0$ *then for all* $y(w)$*,* $U_{y(w)} > 0$*. Further if* $U_{x(w)} > 0$ *then* $U_{y(w)} < 0$ *for* $x(w), y(w)$*.*

For the induction step, suppose the result holds for $n = n-1$*. Let vertices belong to level* $n-1$ *is* $x(w_1), x(w_2), \ldots, x(w_{2^{n-2}}), y(w_1), y(w_2), \ldots, y(w_{2^{n-2}})$*, where* $w_j \in \Sigma_1^{\leq n}$ *and* $|w_j| = n-2$ *and* $j = 1, \ldots, 2^{n-2}$*. Then we have,* $x(w_{j+k}) = x(w_{j+k+1})$ *and* $y(w_{j+k}) = y(w_{j+k+1})$ *for* $j = 1, \ldots, 2^{n-3}$ *and* $k = 0, \ldots, 2^{n-3}-1$*. Now consider the double tree with level* n*. Then the new vertices are added to the bottom level and the degrees of vertices in the level* $n-1$ *change to* α*.*

Let vertices belong to the level n *is* $\{x(w_ju_1) \mid 1 \leq j \leq 2^{n-2}\} \cup \{x(w_ju_2) \mid 1 \leq j \leq 2^{n-2}\} \cup \{y(w_ju_1) \mid 1 \leq j \leq 2^{n-2}\} \cup \{y(w_ju_2) \mid 1 \leq j \leq 2^{n-2}\}$*, where* $u_1, u_2 \in \{0,1\}$*,* $u_1 \neq u_2$*,* $w_j \in \Sigma_1^{\leq n}$ *and* $|w_j| = n-1$*. Then the bottom level of the double tree satisfy the following system of equations.*

$$-\frac{1}{\sqrt{\alpha}}U_{x(w_j)} + U_{x(w_ju_1)} = \lambda_2 U_{x(w_ju_1)}, \tag{4.5.25}$$

$$-\frac{1}{\sqrt{\alpha}}U_{x(w_j)} + U_{x(w_ju_2)} = \lambda_2 U_{x(w_ju_2)}, \tag{4.5.26}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(w_j)} + U_{y(w_ju_1)} = \lambda_2 U_{y(w_ju_1)}, \tag{4.5.27}$$

$$-\frac{1}{\sqrt{\alpha}}U_{y(w_j)} + U_{y(w_ju_2)} = \lambda_2 U_{y(w_ju_2)}, \tag{4.5.28}$$

where $j = 1, \ldots, 2^{n-2}$*. Let* $x(w_i^*), y(w_i^*), (i = 1, \ldots, 2^{n-3}), w^* \in \Sigma_1^{\leq n}$ *are the vertices belong to the level* $n-2$*. Then the vertex* w_1 *satisfy the following equation.*

$$-\frac{1}{\alpha}U_{x(w_1^*)} - \frac{1}{\sqrt{\alpha}}U_{x(w_1u_1)} - \frac{1}{\sqrt{\alpha}}U_{x(w_1u_2)} + U_{x(w_1)} = \lambda_2 U_{x(w_1)}. \tag{4.5.29}$$

The vertex w_2 *satisfy the following equation.*

$$-\frac{1}{\alpha}U_{x(w_1^*)} - \frac{1}{\sqrt{\alpha}}U_{x(w_2u_1)} - \frac{1}{\sqrt{\alpha}}U_{x(w_2u_2)}U_{x(w_2)} = \lambda_2 U_{x(w_2)}. \tag{4.5.30}$$

We can extend this for all vertices in the level $n-1$*. By solving above system of Equations 4.5.25 and 4.5.26, we have* $x(w_ju_1) = x(w_ju_2)$ *and* $y(w_ju_1) = y(w_ju_2)$ *for* $j = 1, \ldots, 2^{n-1}$*. By solving Equation 4.5.29 and Equation 4.5.30 with Equation 4.5.25 and Equation 4.5.26, we have* $x(w_{j+k}) = x(w_{j+1+k})$ *for* $j = 1, \ldots, 2^{n-3}$ *and* $k = 0, \ldots, 2^{n-3}-1$*. From the induction step, if* $x(\epsilon) > 0$ *then* $x(w_j) > 0$ *for* $j = 1, \ldots, 2^{n-3}$ *and if* $x(w_j) > 0$ *then* $y(w_j) < 0$*. Now we have* $x(w_{j+k}) = x(w_{j+1+k})$*. Since* $\lambda_2 \leq \frac{2}{2^{n+1}-3}$*, we have* $x(w_ju_1) > 0$ *and* $x(w_ju_2) > 0$ *for* $j = 1, \ldots, 2^{n-2}$*. Similar result holds for* $y(w_ju_1)$ *and* $y(w_ju_2)$*. Hence the result is true for any* $n \in \mathbf{Z}^+$ *by mathematical induction.* ■

Proposition 4.15
For a double tree DT_n, $Mcut(DT_n) = Lcut(DT_n)$.

(Proof) $Mcut(DT_n)$ bipartition the graph through their roots. By the Proposition 4.14, the second eigenvector of DT_n bipartition the graph by cutting through their roots. Hence $Mcut(DT_n) = Lcut(DT_n)$. ■

4.6 Conclusion

We compare spectral clustering with normalized cut and identify some graphs which perform poorly on spectral methods. Specially we give counter example graphs, where $Mcut(G)$ and $Lcut(G)$ produce different clusters. Double tree is an exception for this since it always have $Mcut(DT_n) = Lcut(DT_n)$. We also noticed that the second eigenvector of $R_{2k,k}$ is an odd vector and it is remained for the future to give a mathematical proof for this. Further we want to consider real world networks and apply the clustering methods by eliminating the subgraphs, which have the same property as we identified here. This is an experimental work remained for the future.

5 Laplacian energy of directed graphs

5.1 Introduction

In this chapter, we address the problem of finding directed graphs with minimum Laplacian energy. First we define Laplacian energy of directed graphs using sum of squares of eigenvalues of directed difference Laplacian matrices. Then we obtain a formula for Laplacian energy of simple directed graphs. Next we enumerate the structure of directed graphs belongs to the class $P(\alpha)$*, where* $\alpha \in Z^+$*. We analyze MMO algorithm introduced by Asahiro, 2006 for minimizing maximum outdegree and investigate the appropriateness of MMO to our problem of minimizing Laplacian energy and give counter examples, where this algorithm is failed. Then we consider the problem by using bipartite semi-matching and find the optimal oriented graph with minimum Laplacian energy. In this chapter, we use* $d(i)$ *to represent the degree of a vertex* i*, instead of using* d_i*.*

5.2 Laplacian energy of undirected graphs.

Gutman et al.[22] defined Laplacian energy of an undirected graph $G = (V(G), E(G))$ *as* $LE_g(G) = \sum_{i=1}^{n} |\mu_i - 2m/n|$*, where* $|V(G)| = n, |E(G)| = m$ *and* μ_i *are the eigenvalues of difference Laplacian matrix.*

Definition 5.1
Let $G = (V(G), E(G))$ *be an undirected graph with* $|V(G)| = n, |E(G)| = m$*. We define* $M(G) = m + \frac{1}{2}\sum_{i=1}^{n}(d(i) - \frac{2m}{n})^2$*, where* $d(i)$ *is the degree of the vertex* i*.*

Theorem 5.1 (Gutman et al.[22])
Let $G = (V(G), E(G))$ *be an undirected graph with* $|V(G)| = n$*. Then*

$$LE_g(G) \quad \leq \quad \sqrt{2M(G)n}. \tag{5.2.1}$$

■

Theorem 5.2 (Gutman et al.[22])
Let $G = (V(G), E(G))$ *is an undirected graph with one component and* $|V(G)| = n, |E(G)| = m$*. Then*

$$LE_g(G) \quad \leq \quad \frac{2m}{n} + \sqrt{(n-1)\left(2M(G) - (\frac{2m}{n})^2\right)}. \tag{5.2.2}$$

■

Theorem 5.3 (Gutman et al.[22])
Let $G = (V(G), E(G))$ *is an undirected graph. Then*

$$2\sqrt{M(G)} \leq \quad LE_g(G) \leq 2M(G). \tag{5.2.3}$$

■

Total π-electron energy and Laplacian energy was compared by Radenković and Gutman [41]. A similar problem for the usual Laplacian energy has been considered by Lazić [28] for undirected graphs using the second spectral moment. According to Lazić [28], Laplacian energy was defined as $LE_l(G) = \sum_{i=1}^{n} \mu_i^2$, where μ_i are the eigenvalues of undirected difference Laplacian matrix. We list some of their results.

Theorem 5.4 ([28])
For any undirected graph G on n vertices whose degrees are $d(1), d(2), \ldots, d(n)$, $LE_l(G) = \sum_{i=1}^{n} d(i)(d(i)+1)$.

■

Theorem 5.5 (Lazić [28])
For any undirected connected graph G on $n \geq 2$ vertices,

$$LE_l(G) \geq 6n - 8. \tag{5.2.4}$$

Equality holds iff G is a path P_n on n vertices. ■

Theorem 5.6 (Lazić [28])
For any $\alpha > 4$, the class $P(\alpha)$ of all non-isomorphic connected graphs with the property $LE_l(G) \leq \alpha$ is finite.

■

By using eigenvalues of difference Laplacian matrix, Laplacian Estrada index was defined by Li et al.[30] and derived some upper and lower boundaries. Further Gutman et al.[21], discussed various properties of energy using incidence matrix. Adiga et al.[2] introduced skew Laplacian energy for directed graphs as $SLE(G) = \sum_{i=1}^{n} \mu_i^2$, where μ_i are the eigenvalues of skew Laplacian matrix $SL(G) = D - S(G)$. $S(G)$ is the adjacency matrix with $s_{ij} = 1$ and $s_{ji} = -1$, whenever there is a arc from $i \rightarrow j$ and 0 otherwise. D is a diagonal matrix with $D(i,i) = d(i) = d^{out}(i) + d^{in}(i)$, where $d^{out}(i)$ is the outdegree and $d^{in}(i)$ is the indegree of a vertex i. By using the definition of Gutman et al.[22], Adiga et al.[2] obtained upper and lower bounds to the Laplacian energy of simple directed graphs similar to the Equation 5.2.1, Equation 5.2.2 and the Equation 5.2.3. We list them in the Equation 5.2.7, Equation 5.2.8 and the Equation 5.2.9. Skew Laplacian eigenvalues satisfy the following relations.

$$\sum_{i=1}^{n} \mu_i = 2m, \tag{5.2.5}$$

$$\sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} d(i)(d(i)-1). \tag{5.2.6}$$

Theorem 5.7 (Adiga et al.[2])
Let $G = (V(G), E(G))$ be a directed graph with $|V(G)| = n$ and $|E(G)| = m$. Let $SLE(G)$ be the skew Laplacian energy of G and $M_1 = M + 2m = m + \frac{1}{2}\sum_{i=1}^{n}(d(i) - \frac{2m}{n})^2$. Then

$$SLE(G) \quad \leq \quad \sqrt{2M_1 n}. \tag{5.2.7}$$

If G has k components then,

$$SLE(G) \quad \leq \quad k + \sqrt{(n-1)(2M_1 - k^2)}, \text{ and} \tag{5.2.8}$$

$$2\sqrt{M} \leq \quad SLE(G) \quad \leq 2M_1. \tag{5.2.9}$$

5.3 Laplacian energy of directed graphs

Let $D = diag(d^{out}(1), d^{out}(2), d^{out}(3), \ldots, d^{out}(n))$ be a diagonal matrix whose diagonal entries are the outdegrees of the vertices $v_1, v_2, \ldots, v_n$. Then we called $L(G) = D(G) - A(G)$, the difference Laplacian matrix of a directed graph and its eigenvalues are denoted by $\{\mu_1, \mu_2, \ldots, \mu_n\}$. Since $L(G)$ is an asymmetric matrix it does not give always real eigenvalues.

Definition 5.2 (Laplacian energy of directed graphs)
Let $G = (V(G), E(G))$ be a directed graph. Then Laplacian energy of G is defined as $LE(G) = \sum_{i=1}^{n} \mu_i^2$, where $|V(G)| = n$ and $\mu_i, (i = 1, \ldots, n)$ are the eigenvalues of the difference Laplacian matrix.

The eigenvalues of Laplacian matrices of directed graphs are sometimes complex and appeared as conjugate pairs. Sometimes our definition may be confused with other definitions. The following we provide some examples to explain this difference. It shows that the sum of squares of absolute values of Laplacian eigenvalues are different from the sum of squares of eigenvalues, when eigenvalues are complex values.

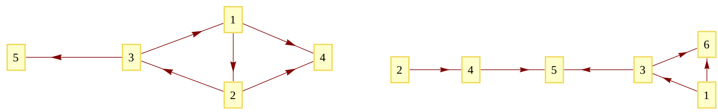
Example 5.1
The eigenvalues of the graph shown in the Figure 21(a) are $\{0, 0, 1, \frac{(5 - \mathbf{i}\sqrt{3})}{2}, \frac{(5 + \mathbf{i}\sqrt{3})}{2}\}$.

$$\sum_{i=1}^{n} |\mu_i|^2 = \sum_{i=1}^{n} \mu_i.\bar{\mu_i} \quad = \quad 15,$$
$$LE(G) = \sum_{i=1}^{n} \mu_i^2 \quad = \quad 12.$$

Example 5.2
The eigenvalues of the graph shown in the Figure 21(b) are $\{0, 0, 1, 1, 2, 2\}$.

$$\sum_{i=1}^{n} |\mu_i|^2 = \sum_{i=1}^{n} \mu_i.\bar{\mu_i} \quad = \quad 10,$$
$$LE(G) = \sum_{i=1}^{n} \mu_i^2 \quad = \quad 10.$$

If G has complex eigenvalues then $\sum_{i=1}^{n} \mu_i^2 < \sum_{i=1}^{n} |\mu_i|^2$. *If G has real eigenvalues then both quantities are equal.*



(a) G_1 (b) G_2

Figure 21: Graphs with real and complex eigenvalues.

Theorem 5.8
If G is a disconnected directed graph with components $G_1, G_2, \ldots, G_n$,

$$LE(G) \quad = \quad \sum_{i=1}^{n} LE(G_i). \tag{5.3.1}$$

Theorem 5.9
Let $G = (V(G), E(G))$ be a directed graph with vertex degrees $(d^{out}(1), d^{out}(2), \ldots, d^{out}(n))$. If G is a simple directed graph then

$$LE(G) = \sum_{i=1}^{n} (d^{out}(i))^2$$

If G is a symmetric directed graph then

$$LE(G) = \sum_{i=1}^{n} d^{out}(i)(d^{out}(i) + 1).$$

(Proof) Suppose G is a simple directed graph. Let D be a diagonal matrix with $D(i,i) = d^{out}(i)$, where $i \in V(G)$. If $i \to j$ is an arc then $a_{ij} = 1$ and $a_{ji} = 0$. From Viéte Rule, it is clear that $\sum_{i=1}^{n} \mu_i = Trace(L(G)) = \sum_{i=1}^{n} d^{out}(i)$ *and the sum of the determinant of all 2×2 principal sub matrices are* $\sum_{i<j} \mu_i \mu_j$.
That is

$$\begin{aligned} \sum_{i<j} \mu_i \mu_j &= \sum_{i<j} det \begin{pmatrix} d^{out}(i) & -a_{ij} \\ 0 & d^{out}(j) \end{pmatrix} \\ &= \sum_{i<j} d^{out}(i) d^{out}(j). \end{aligned}$$

For every $i < j$,

$$\begin{aligned}\sum_{i \neq j} \mu_i \mu_j &= 2\sum_{i<j} \mu_i \mu_j \\ &= 2\sum_{i<j} d^{out}(i) d^{out}(j) \\ &= \sum_{i \neq j} d^{out}(i) d^{out}(j).\end{aligned}$$

Therefore

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} \mu_i^2 = (\sum_{i=1}^{n} \mu_i)^2 - \sum_{i \neq j} \mu_i \mu_j && (5.3.2) \\ &= (\sum_{i=1}^{n} d^{out}(i))^2 - (\sum_{i \neq j} d^{out}(i) d^{out}(j)) && (5.3.3) \\ &= \sum_{i=1}^{n} (d^{out}(i))^2. && (5.3.4)\end{aligned}$$

If G is a symmetric directed graph then $d^{out}(i) = d^{in}(i) = d(i)$ for each vertex i. Hence Laplacian energy of G is similar to the Laplacian energy of undirected graph which is given as $LE(G_l) = \sum_{i=1}^{n} d(i)(d(i)+1)$ in [28]. We can replace $d(i)$ with $d^{out}(i)$ and obtained the required result. ■

Corollary 5.1
For any simple connected directed graph G, its Laplacian energy $LE(G)$ is an integer.

(Proof) Since the degree of a vertex is an integer, their sum of squares is also an integer. Hence

$$LE(G) = \sum_{i=1}^{n} (d^{out}(i))^2,$$

is an integer. ■

Corollary 5.2
The Laplacian energy of a simple directed path P_n with $n \geq 2$ is $(n-1)$.

(Proof) Since every simple directed path P_n has exactly $(n-1)$ vertices with outdegree 1 and one vertex with degree 0, $LE(P_n) = (n-1)$ by the Theorem 5.9. ■

Corollary 5.3
The Laplacian energy of a simple directed cycle C_n with $n \geq 3$ is n.

(Proof) Since every vertex in C_n has outdegree one, this follows from the Theorem 5.9. ■

Corollary 5.4
For any connected directed graph on $n \geq 2$ vertices, we have,

$$n-1 \leq LE(G) \leq n^2(n-1) \tag{5.3.5}$$

Moreover, $LE(G) = n^2(n-1)$ if and only if G is a complete directed graph K_n and $LE(G) = n-1$ if and only if G is a directed path P_n on n vertices.

(Proof) Let G be a connected directed graph with $n \geq 2$ vertices. Maximum degree of any vertex is less than or equal to $(n-1)$. If G is a simple connected graph then $LE(G) = \sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} (d^{out}(i))^2 < \sum_{i=1}^{n} d^{out}(i)(d^{out}(i)+1)$.

If G is a symmetric directed graph then $LE(G) = \sum_{i=1}^{n} d^{out}(i)(d^{out}(i)+1) \leq n^2(n-1)$. This implies that for any directed graph G, $LE(G) \leq n^2(n-1)$. Since each vertex of a complete directed graph has degree $n-1$, it is clear that the complete directed graph K_n has the maximum Laplacian energy among directed graphs of n vertices. We prove left side of the inequality 5.3.5 by induction. As we know, to form a directed graph, we need at least two vertices. Only connected graph which has two vertices is a simple or a bidirected path. Since eigenvalues of $L(P_2) = \left(\begin{smallmatrix} 1 & -1 \\ 0 & 0 \end{smallmatrix}\right)$ is 1 and 0 and $L(K_2) = \left(\begin{smallmatrix} 1 & -1 \\ -1 & 1 \end{smallmatrix}\right)$ is 2 and 0, the result is true for $n = 2$. Suppose the result is true for any connected directed graph with $n-1$ vertices. That is $LE(G) \geq n-2$. Then we need to prove the result for any arbitrary connected directed graph with n vertices. Let G be a connected directed graph with n vertices. Then, there is an induced subgraph $H \subset G$ on $n-1$ vertices which is also connected. Let $V(H) = \{v_1, v_2, \ldots, v_{n-1}\}$, $V(G) = V(H) \cup \{v_n\}$ and $LE(H) \geq n-2$. It is easy to show that $LE(G) \geq LE(H)+1$. So we have $LE(G) \geq n-1$. We can also prove that if G is a simple, connected directed graph with n vertices such that $LE(G) = n-1$, then G must be a directed path P_n. Suppose $LE(G) = n-1$. Let $n = 2$. Then $LE(G) = 1$. Since $LE(G) = \sum_{i=1}^{2} (d^{out}(i))^2$, we have $d^{out}(1) + d^{out}(2) = 1$. This happened when we have a one vertex with outdegree 1. That is there exists a one directed edge between two vertices. Therefore G should be a directed path. ■

5.4 Relationship between undirected graphs and directed graphs

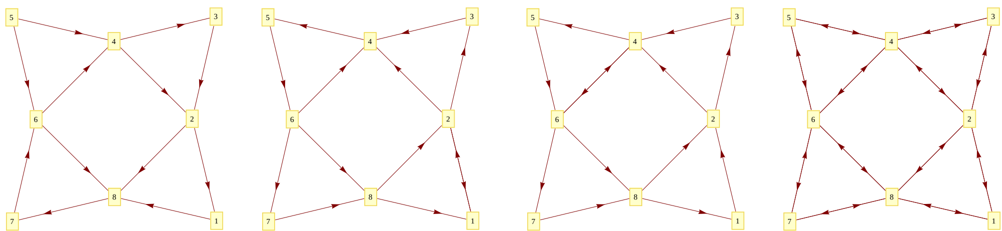
This section explains the relationship between undirected and directed graphs. Every undirected graph can be converted to a directed graph by assigning directions. If each edge is replaced by two way directions then it is similar to the undirected graph.

Definition 5.3
For a given directed graph $G_d = (V_d, E_d)$, we define an undirected graph $U(G_d) = (U(V_d), U(E_d))$ by $U(V_d) = V_u$ and $U(E_d) = \{(v_1, v_2) \mid (v_1, v_2) \in E_d \text{ or } (v_2, v_1) \in E_d\}$.

Let $A(U(G)) = (a_{ij})$ be the adjacency matrix of $U(G)$ and let $A'(G) = (a'_{ij})$ be the adjacency matrix of G. Then

$$a_{ij} = \begin{cases} 1 & \text{if } a'_{ij} = 1 \text{ or } a'_{ji} = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Example 5.3
The Figure 22 shows four directed graphs $G_{d_1}, G_{d_2}, G_{d_3}, G_{d_4}$ with $U(G_{d_i}) = G_u$. The $LE(G_{d_i})$ have different Laplacian energies.



(a) G_{d_1} (b) G_{d_2} (c) G_{d_3} (d) G_{d_4}

Figure 22: Directed graphs for a given undirected graph.

Theorem 5.10
For any directed graph G_d, $LE(G_d) \leq LE_l(U(G_d))$

(Proof) Let $G_d = (V_d, E_d)$ and $U(G_d) = (V_u, E_u)$. For any vertex $v \in V_d$, $d^{out}(v) \leq d(v)$.

$$\begin{aligned}
LE_l(U(G_d)) &= \sum_{i=1}^{n} d(i)(d(i)+1) \\
&= \sum_{i=1}^{n} d(i)^2 + \sum_{i=1}^{n} d(i) \\
&\geq \sum_{i=1}^{n} (d^{out}(i))^2 + \sum_{i=1}^{n} d^{out}(i) \\
&\geq LE(G_d).
\end{aligned}$$

Equality occur if and only if G_d is a symmetric directed graph. ■

Theorem 5.11
Let G be a directed graph and $G' = G - e$ be a directed graph obtained by deleting arc e. Then $LE(G') < LE(G)$.

(Proof) Let $G = (V_d, E_d)$ be a directed graph with $|V_d| = n$. Let $H = (V_h, E_h)$ be an edge induced sub graph with $|V_h| = n_1$ and $E_h = e$. Define G' as $H \oplus (n - n_1)K_1$. Then the directed difference Laplacian matrix $L(G)$ of G is the $L(G - E_h) + L(G')$. $L(G')$ is a square matrix with maximum eigenvalue 1 and all other 0. This implies that there exists at least one vertex i such that $\mu_i(G) \geq \mu_i(G')$ and then we have $\sum_{i=1}^{n} \mu_i^2(G) > \sum_{i=1}^{n} \mu_i^2(G')$. Thus the theorem holds. ■

Proposition 5.1
Let G_d be a non-symmetric directed graph with $U(G_d) = G_u$. Then there exists a directed graph G'_d such that $U(G'_d) = G_u$ and $LE(G_d) < LE(G'_d)$.

(Proof) Let G_d be a non-symmetric directed graph. Then there exists $(v_i, v_j) \in E(G_u)$ and $(v_i, v_j) \notin E(G_d)$ or $(v_j, v_i) \notin E(G_d)$. Suppose $(v_i, v_j) \notin E(G_d)$. Let G'_d be a connected directed graph with $V(G'_d) = V(G_d)$, $E(G'_d) = E(G_d) \cup (v_i, v_j)$. Then $U(G'_d) = G_u$ and by the Theorem 5.11, $LE(G'_d) > LE(G_d)$. By adding arcs for each vertex we can transform given non-symmetric graph to the symmetric graph, which is identical to the undirected graph. ■

Proposition 5.2
Let G_d be a non-simple directed graph with $U(G_d) = G_u$. Then there exists a directed graph G'_d such that $U(G'_d) = G_u$ and $LE(G_d) > LE(G'_d)$.

(Proof) Suppose G_d be a non-simple directed graph. Then there exists $(v_i, v_j) \in E(G_u)$ and $(v_i, v_j) \in E(G_d)$ and $(v_j, v_i) \in E(G_d)$. Suppose $(v_i, v_j) \in E(G_d)$. Let G'_d be a connected directed graph with $V(G'_d) = V(G_d)$ and $E(G'_d) = E(G_d) - (v_i, v_j)$. Then $U(G'_d) = G_u$ and by the Theorem 5.11, $LE(G'_d) < LE(G_d)$. By deleting arcs from each vertex we can transform given non-simple directed graph to a simple directed graph. ■

Theorem 5.12
Let $P(\alpha) = \{G \mid LE(G) \leq \alpha,\ G : a\ simple\ connected\ \ directed\ graph\}$. For any $\alpha \geq 1$, the class $P(\alpha)$ of all non-isomorphic connected directed graphs with the property $LE(G) \leq \alpha$ is finite.

(Proof) Let G be a directed graph with n vertices and m arcs such that $LE(G) \leq \alpha$. By the Corollary 5.4, $n - 1 \leq LE(G) \leq \alpha$. Hence we obtain $n - 1 \leq \alpha$. Since n is finite, class $P(\alpha)$ is also finite.
■

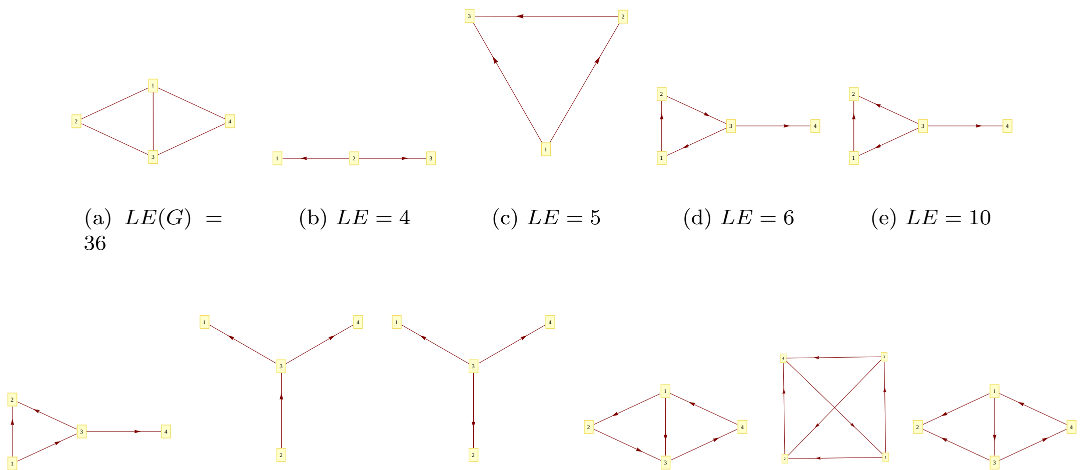
Corollary 5.5
The class $P(10)$ contains exactly 47 directed graphs. More exactly 29 directed graphs with $n \leq 10$, 8 directed cycles with $n \leq 10$ and 10 directed paths with $n \leq 11$. Some of the graphs are listed in the Figure 23 and the Figure 24.

(Proof) Let $\alpha = 10$. Every simple connected directed graph with n vertices has at least $(n-1)$ arcs. Notice that for $n = 12$, $LE(G) \geq (n-1) = 11 > 10$. For $n = 11$, $LE(G) \geq 10$. Therefore all directed graphs of the class $P(10)$ have at most 11 vertices. Since $LE(P_n) = n - 1$ it has 10 directed paths P_n with $n \leq 11$ and since $LE(C_n) = n$ it has 8 directed cycles with $n \leq 10$. ■

Theorem 5.13
Let $G = (V_d, E_d)$ be a simple connected directed graph with $|V_d| = n$ and $|E_d| = m$. If $\triangle = \max\{d^{out}(v) \mid v \in V_d\}$ and $\delta = \min\{d^{out}(v) \mid v \in V_d\}$ then

$$\frac{m^2}{n} \leq LE(G) \leq m(\triangle + \delta) - n\delta\triangle.$$

(Proof) First we will prove the left hand side of the inequality. By Cauchy Schwarz inequality, $LE(G) = \sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n} (d^{out}(i))^2 \geq \frac{1}{n}\left(\sum_{i=1}^{n} d^{out}(i)\right)^2 = \frac{m^2}{n}$. Next consider the right hand side of



(a) $LE(G) = 36$ (b) $LE = 4$ (c) $LE = 5$ (d) $LE = 6$ (e) $LE = 10$

(f) $LE = 8$ (g) $LE = 5$ (h) $LE = 9$ (i) $LE = 7$ (j) $LE = 10$ (k) $LE = 9$

Figure 23: Directed graphs with $n \leq 4$.

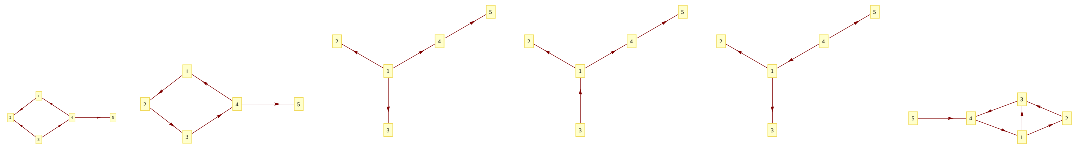
the inequality. Consider $(d^{out}(i)-\delta)(d^{out}(i)-\triangle)$. *For any* i, $(d^{out}(i)-\delta) \geq 0$ *and* $(d^{out}(i)-\triangle) \leq 0$. *Therefore* $(d^{out}(i)-\triangle)(d^{out}(i)-\delta) \leq 0$, *for* $i \in V_d$. *Further* $\sum_{i=1}^{n}(d^{out}(i)-\triangle)(d^{out}(i)-\delta) = \sum_{i=1}^{n}(d^{out}(i))^2 - (\triangle+\delta)\sum_{i} d^{out}(i) + n\delta\triangle \leq 0$. *This shows that* $\sum_{i=1}^{n}(d^{out}(i))^2 \leq m(\triangle+\delta) - n\delta\triangle \leq 0$. *Hence* $LE(G) \leq m(\triangle+\delta) - n\delta\triangle$. ■

Remarks. *If* $\triangle = \delta$ *then* $m = \sum_{i=1}^{n} d^{out}(i) = n\triangle$ *and* $m(\triangle+\delta) - n\delta\triangle = 2n\triangle^2 - n\triangle^2 = n\triangle^2 = \frac{m^2}{n}$.

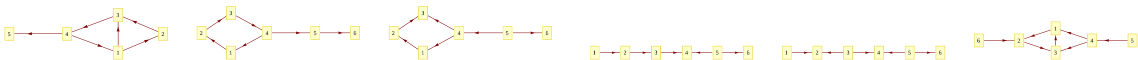
In the next few sections, we consider the existing algorithms for minimizing maximum outdegree of an oriented graph. Similar kind of problems studied in literature are scheduling problems, load balancing problems and network flow problems. First we summarized the exiting results and discuss how far those algorithms can be used to solve our problem.

5.5 Minimizing maximum outdegree algorithms and Laplacian energy

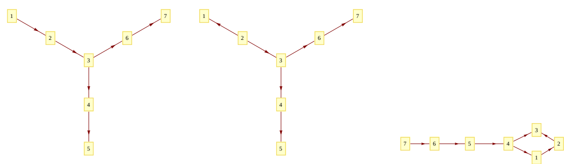
Since Laplacian energy can be represented using the sum of squares of outdegrees, we consider the way of minimizing the sum of squares of outdegrees. In this section, we describe the relationship between minimum Laplacian energy of directed graphs and minimizing maximum outdegree algorithms(MMO).



(a) $LE = 9$ (b) $LE = 7$ (c) $LE = 10$ (d) $LE = 6$ (e) $LE = 8$ (f) $LE = 8$



(g) $LE = 10$ (h) $LE = 8$ (i) $LE = 10$ (j) $LE = 7$ (k) $LE = 9$ (l) $LE = 9$



(m) $LE = 8$ (n) $LE = 10$ (o) $LE = 9$

Figure 24: Directed graphs with $5 \geq n < 10$.

Definition 5.4 (Optimal Laplacian energy)
Let G_u be an undirected graph. The optimal directed Laplacian energy $LE_{opt}(G_u)$ of G_u is defined by, $LE_{opt}(G_u) = \min\{LE(G_d) \mid G_d$ is a directed graph and $U(G_d) = G_u\}$.

Definition 5.5 (Maximum outdegree)
For a directed graph $G_d = (V_d, E_d)$, the maximum outdegree $\triangle(G_d)$ of G_d is defined by $\triangle(G_d) = \max\{d^{out}(v) \mid v \in V_d\}$.

Definition 5.6 (Optimum maximum degree)
Let G_u be an undirected graph. The optimal maximum outdegree $\triangle_{opt}(G_u)$ of G_u is defined by $\triangle_{opt}(G_u) = \min\{\triangle(G_d) \mid G_d$ is a directed graph and $U(G_d) = G_u\}$.

Definition 5.7
Let $G_d = (V_d, E_d)$ be a directed graph. We denote $v \to w$ if $(v, w) \in E_d$. We also denote $v \Rightarrow w$ if there exists $v_1, v_2, \ldots, v_k \in V_d, (k \geq 1)$ such that $v = v_1, v_1 \to v_2, \ldots, v_{k-1} \to v_k$ and $v_k = w$.

Proposition 5.3
Let $G_u = (V_u, E_u)$ be an undirected graph and $G_d = (V_d, E_d)$ be a directed graph satisfying $U(G_d) = G_u$. If $\triangle(G_d) = p$ and $\{d^{out}(v) \mid v \in V_d\} = \{p, p-1\}$ then $LE(G_d) = LE_{opt}(G_u)$.

(Proof) Let $k = |\{v \in V_d \mid d^{out}(v) = p\}|$ and $l = |\{v \in V_d \mid d^{out}(v) = p-1\}|$. Since $\sum\{d^{out}(v) \mid v \in V_d\} = |E_u|$, we have $pk + (p-1)l = |E_u|$. Since $k + l = |V_u|$, k and l can be uniquely determined. $|E_u| = kp + l(p-1) = |V_u|p + (k - |V_u|)$ and $|V_u|p = |E_u| + |V_u| - k$. Hence $p = \dfrac{|E_u|}{|V_u|} + 1 - \dfrac{k}{|V_u|}$. Since $1 \leq k \leq |V_u|$ then $0 \leq 1 - \dfrac{k}{|V_u|} < 1$. So we have $p = \lceil \dfrac{|E_u|}{|V_u|} \rceil$.
Let $h(x_1, x_2, \ldots, x_n, \lambda) = \sum_{i=1}^{n} x_i^2 + 2\lambda(\sum_{i=1}^{n} x_i - |E_u|)$. Since $\dfrac{\partial h}{\partial x_i} = 2x_i + 2\lambda = 0$ and $\dfrac{\partial h}{\partial \lambda} = \sum_{i=1}^{n} x_i - |E_u| = 0$, the function h is minimize at $x_i = -\lambda, (i = 1, \ldots, n)$ and $\sum_{i=1}^{n} x_i = |E_u|$. Since $\sum_{i=1}^{n} x_i = -|V_u|\lambda = |E_u|$, we have $\lambda = -\dfrac{|E_u|}{|V_u|}$ and $x_i = \frac{|E_u|}{|V_u|}, (i = 1, \ldots, n)$. If all x_i are integer, the function h have minimum value for $x_i \in \{\lceil \dfrac{|E_u|}{|V_u|} \rceil, \lceil \dfrac{|E_u|}{|V_u|} - 1 \rceil\}$ for $(i = 1, \ldots, n)$. Taking $x_i = d^{out}(v_i)$, we have $h(x_1, x_2, \ldots, x_n, \lambda) = LE(G_d)$. So $LE(G_d) = kp^2 + l(p-1)^2$ gives the optimal solution. ■

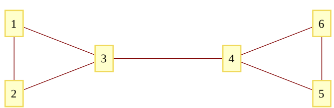
Finding the orientation of a simple directed graph by minimizing maximum outdegree of a vertex is studied in literature by [45] and [5] and is called MMO (minimizing maximum outdegree) algorithms. In order to minimize the maximum outdegree and find a optimal solution to MMO problems, [5] use simple algorithm called reverse algorithm as in the Table 3.

Reverse path cause to decrease the maximum outdegree by one and increase the outdegree of the terminal vertex of path by one. It is proved by [5] that if $G_d = MMO(G_u)$ then $\triangle_{opt}(G_u) = \triangle(G_d)$.

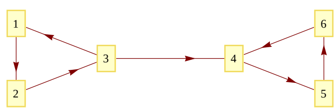
Example 5.4
In the Figure 25, we have two directed graphs G_{d_1} and G_{d_2} with $U(G_{d_1}) = U(G_{d_2}) = G_u$. The maximum outdegree of G_{d_1} and G_{d_2} are same. But $\{d^{out}(v) \mid v \in V_{d_1}\} = \{1, 2\}$ and $\{d^{out}(v) \mid v \in$

Input	An undirected graph $G_u = (V_u, E_u)$.
Output	Oriented graph $MMO(G_u) = G_d = (V_d, E_d)$.
Step 1:	Set $E_d = \emptyset$.
Step 2:	Assign an arbitrary orientation and update E_d.
Step 3:	Compute outdegree $d^{out}(v)$ for each $v \in V_d$. Let u be $\max\{d^{out}(v) \mid v \in V_d\}$.
Step 4:	Find a directed path $P = u \to v_1 \to \cdots \to v_k$ of length $k (k \geq 1)$ which satisfy $d^{out}(v_i) \leq d^{out}(u)$, for $1 \leq i \leq k-1$ and $d^{out}(v_k) \leq d^{out}(u) - 2$. If such P exists then set $E_d = E_d \setminus \{P \cup \bar{P}\}$, where $\bar{P} = v_k \to \cdots \to v_1 \to u$ and goto Step 3. Otherwise halt.

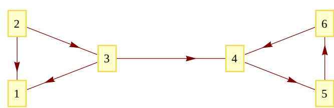
Table 3: MMO Algorithm.



(a) G_u



(b) $LE(G_{d_1}) = 9$



(c) $LE(G_{d_2}) = 11$

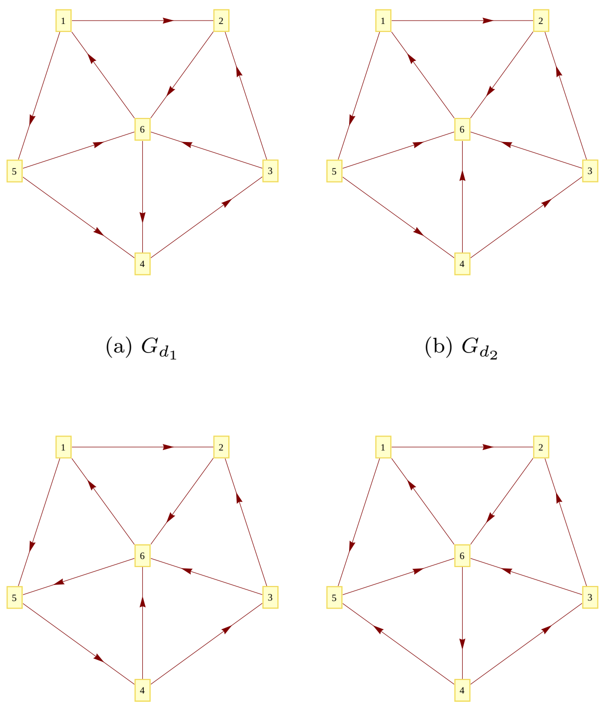
Figure 25: Equal maximum degree and different Laplacian energy.

$V_{d_2}\} = \{0, 1, 2\}$. It is clear that $LE(G_{d_1}) \neq LE(G_{d_2})$. In the Figure 26, we have four directed graphs $G_{d_1}, G_{d_2}, G_{d_3}, G_{d_4}$ with $U(G_{d_i}) = G_u$ and $LE(G_{d_i}) = LE_{opt}(G_u), (i = 1, 2, 3, 4)$. We can see $\{d^{out}(v) \mid v \in V_{d_i}\} = \{1, 2\}$ and $|\{v \in V_{d_i} \mid d^{out}(v) = 1\}| = |\{v \in V_{d_j} \mid d^{out}(v) = 1\}|$ and $|\{v \in V_{d_i} \mid d^{out}(v) = 2\}| = |\{v \in V_{d_j} \mid d^{out}(v) = 2\}|$ for $(i, j = 1, 2, 3, 4)$ and $i \neq j$, which follows the Proposition 5.3.

Proposition 5.4
Let $G_u = (V_u, E_u)$ be an undirected graph and $G_d = (V_d, E_d) = MMO(G_u)$. Let $v_0 \in V_d$ be a vertex with $d^{out}(v_0) = \triangle(G_d)$. Define $V' = \{w \in V_d \mid v_0 \Rightarrow w\}$. $G'_u = (V', E'_u)$ be an induced undirected graph, where $E'_u = \{(u, v) \in E_u \mid u, v \in V'\}$ and $G'_d = (V', E'_d)$ be a directed graph, where $E'_d = \{(u, v) \in E_d \mid u, v \in V'\}$. Then the following relations hold.

1. $d^{out}(v_0) \geq d^{out}(v') \geq d^{out}(v_0) - 1$ *for* $v' \in V'$.
2. $LE(G'_d) = LE_{opt}(G'_u)$

(Proof)



(a) G_{d_1} (b) G_{d_2}

(c) G_{d_3} (d) G_{d_4}

Figure 26: Oriented graphs with minimum Laplacian energy.

1. *Let $v' \in V'$. Then we have a path $P = v_0 \to \cdots \to v'$ from v_0 to v'. Since $d^{out}(v_0) = \triangle(G_d)$, we have $d^{out}(v') \leq d^{out}(v_0)$. Further $G_d = MMO(G_u)$ implies that $d^{out}(v') > d^{out}(v_0) - 2$. Therefore $d^{out}(v') \geq d^{out}(v_0) - 1$.*

2. *From the part 1, we have $\{d^{out}(v) \mid v \in V'\} = \{d^{out}(v_0), d^{out}(v_0) - 1\}$.*

   By the Proposition 5.3, we have $LE(G'_d) = LE_{opt}(G'_u)$.

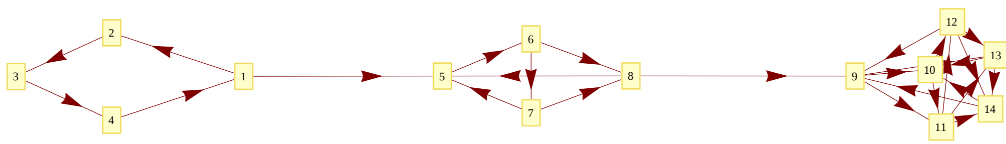
■

Theorem 5.14
Let $G_u = (V_u, E_u)$ be an undirected graph and $G_d = (V_d, E_d) = MMO(G_u)$. Let $p = \triangle(G_d), V_p = \{v \in V_d \mid d^{out}(v) = p\}$ and $V_1 = \{w \in V_d \mid v_p \in V_p, v_p \Rightarrow w\}$. If $V_u = V_1$ then $LE(G_d) = LE_{opt}(G_u)$.

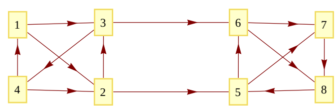
(Proof) Since $G_d = MMO(G_u)$ then $\{d^{out}(v) \mid v \in V_1\} = \{p, p-1\}$. If $V_u = V_1$ then we have $LE(G_d) = LE_{opt}(G_u)$ by the Proposition 5.3. ■

Example 5.5

In the Figure 27(a), $MMO(G_u) = (V_d, E_d)$ and $\{d^{out}(v) \mid v \in V_d\} = \{3, 2, 1\}$. $p = \triangle(G_d) = 3, V_p = \{9, 11, 12\}, V_1 = \{9, 10, 11, 12, 13, 14\}$. So we cannot apply the Theorem 5.14. In the Figure 27(b) $MMO(G_u) = (V_d, E_d)$ and $\{d^{out}(v) \mid v \in V_d\} = \{2, 1\}$. Here $p = \triangle(G_d) = 2$, $V_p = \{1, 2, 3, 4, 5, 6\}$ and $V_1 = \{1, 2, 3, 4, 5, 6, 7, 8\}$. Then we have $LE(MMO(G_u)) = LE_{opt}(G_u)$ from the Theorem 5.14. However, we note that both graphs have optimal orientation and minimum Laplacian energy.



(a) $MMO(G_u)$



(b) $MMO(G_u)$

Figure 27: Graphs consists of optimal Laplacian Energy.

Example 5.6

The counter example graphs, where we could not find an optimal orientation using MMO are shown in the Figure 28 and the Figure 29. Let $G_1 = (V_{d_1}, E_{d_1})$ be a directed graph as in the Figure 28. Then we have $\{d^{out}(v) \mid v \in V_{d_1}\} = \{5, 4, 3, 2\}$. There does not exist a directed path from maximum degree 5 to degree 3 or 2. In other words vertices $\{1, 2, 3, 4, 5, 6\}$ cannot access from the vertices $\{7, 8, 9, 10, 11, 12, 13, 14, 15, 16\}$. Reverse path algorithm of MMO halt at this stage, since there is no directed path start from maximum vertex degree. However, the graph G_1 is not optimal since we can still change some arcs and change the outdegrees of vertices. The Figure 29 also demonstrate a worst case example, where minimum degree vertex v_2 can not access from the maximum degree vertex v_8, and it is impossible to continue MMO algorithm. Hence there are some zero degree vertices remained.

Reverse path algorithm always starting from maximum degree vertex and find a directed path in order to reduce the maximum outdegree. Even the maximum degree is reduced, there is no effect to the outdegree of a minimum degree vertex if there is no directed path exists from the maximum degree to the minimum degree. This algorithm works well if graph has only two consecutive degrees as described in the Proposition 5.3 of previous section. However, this algorithm is not always efficiently minimize the sum of squares of outdegrees. This can be modified by considering the semi matching problem.

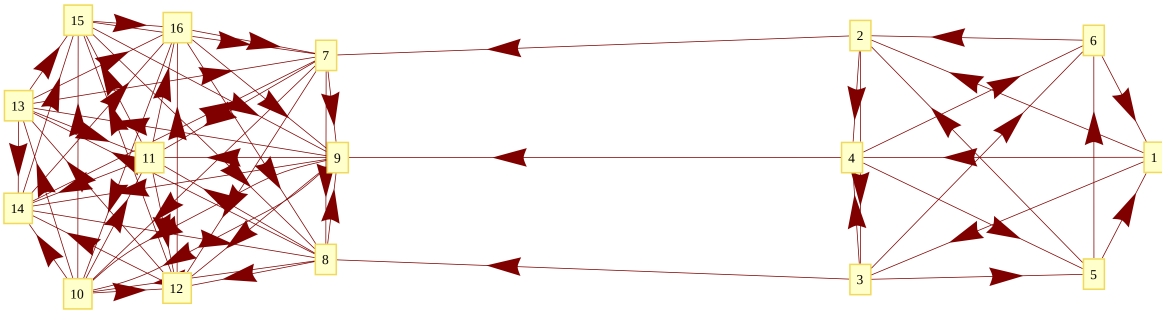


Figure 28: Worst case example(1).

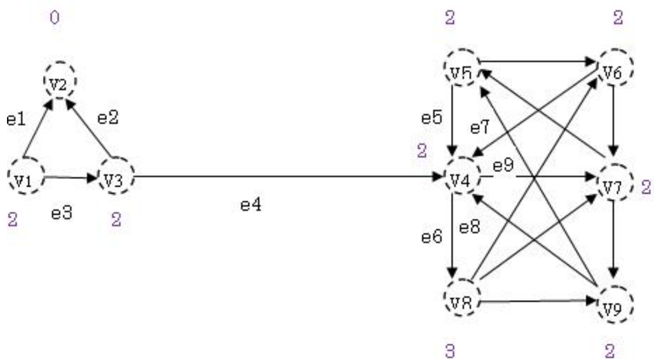


Figure 29: Worst case example(2).

5.6 Find an oriented graph with minimum Laplacian energy using semi-matchings

In this section, we solve our problem using optimal semi-matching problem. First we will present previous results in [23] related to the bipartite semi-matchings.

5.7 Characterization of optimal semi matchings

Definition 5.8 (Semi matching)
Let $G = (U, V, E)$ be a bipartite graph. A set $M \subseteq E(G)$ be a semi-matching if each vertex $u \in U(G)$ is incident with exactly one edge in $E(G)$.

We denote the degree of a vertex v with respect to the semi matching M as $d_M(v)$. In the load balancing problem, $d(v)$ denote the number of tasks that machine v is capable of executing and $d_M(v)$ is the number of tasks assigned to machine v. This is called the load on vertex v.

Definition 5.9 (Cost of a vertex with respect to semi-matching)
Let $G = (U, V, E)$ be a bipartite graph with $|V| = m$ and $|U| = n$ The cost of a semi-matching with respect to the vertex v is $cost_M(v) = \sum_{i=1}^{d_M(v)} i = \dfrac{(d_M(v)+1)d_M(v)}{2}$ and the total cost of a semi-matching is $T(M) = \sum_{i=1}^{n} cost_M(v_i)$

A semi-matching with minimum cost is called an **optimal semi-matching**.

Definition 5.10 (Alternate path)
Let M is a semi matching in a bipartite graph $G = (U, V, E)$. Then alternate path is a sequence of edges $P = ((v_1, u_1), (u_1, v_2), \ldots, (u_{k-1}, v_k))$ with $v_i \in V, u_i \in U$ and $(v_i, u_i) \in M$ for each i.

Definition 5.11 (Cost reducing path)
*Let M be a semi matching and
$P = ((v_1, u_1), (u_1, v_2), \ldots, (u_{k-1}, v_k))$ be an alternate path where, $v_i \in V, u_i \in U$, and $(v_i, u_i) \in M$. If $d_M(v_1) - 1 > d_M(v_k)$ then P is called a cost reducing path relative to M. The cost reduce path can be eliminated by deleting edges (v_i, u_i) from M for all i and adding (u_i, v_{i+1}) to M for all i. Then the cost of vertex v_1 decrease by 1 and the cost of vertex v_k increase by 1.*

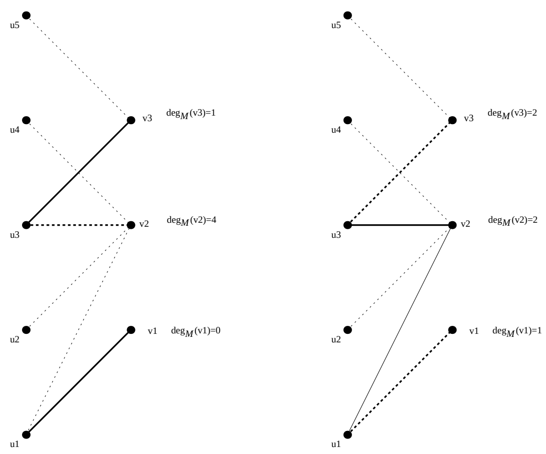
Optimal semi-matchings have useful load balancing such as minimum variance of $d_M(v)$, minimum maximum $d_M(v)$ and minimum L_p norm of $d_M(v)$.

Example 5.7 (Cost reducing path)
Let $G = (U, V, E)$ be a bipartite graph such that $V = \{v_1, v_2, v_3\}$, $U = \{u_1, u_2, u_3, u_4, u_5\}$ and $E = \{(u_1, v_1), (u_1, v_2), (u_2, v_2), (u_3, v_2), (u_4, v_2), (u_3, v_3), (u_5, v_3)\}$. We define semi matching M such that $M = \{(u_1, v_2), (u_2, v_2), (u_3, v_2), (u_4, v_2), (u_5, v_3)\}$. The Figure 30(a) shows the graph with semi matching M. We use dotted lines to represent the semi matching. Vertex v_2 has load 4 and vertex v_3 has load 1 and v_1 has load 0 with respect to the semi matching M. There exists an alternating path $\{(v_2, u_1), (u_1, v_1)\}$ in G, which is a cost reducing path and we can reduce the cost on degree v_2 by deleting edge (v_2, u_1) from M and adding (u_1, v_1) to M. This will increase $d_M(v_1)$ by 1 and decrease $d_M(v_2)$ by 1. Similarly, $(v_2, u_3), (u_3, v_3)$ is a cost reducing path and we can balance the cost by deleting edges (v_2, u_3) from M and add (u_3, v_3) to M. Then we can obtain the graph with optimal semi matching as shown in the Figure 30(b).

Theorem 5.15 ([23])
Semi-matching is optimal if and only if no cost reducing path exists.

Theorem 5.16 ([23])
Let $1 < p < \infty$. A semi-matching is optimal if and only if it is optimal with respect to the L_p norm of its load vector.

(Proof) Fix any $p > 1$ and define $f_p(x) = x^p$. f_p is strictly convex and $cost_M(f_p)$ is a strict cost function. Let X be the load vector for M. Since $\parallel X \parallel_p = (cost_M(f_p(x)))^{1/p}$, M optimizes $\parallel X \parallel_p$ if and only if it optimizes $cost_M(f_p(x))$. That is if and only if M is an optimal semi matching. ■



(a) Semi matching (b) Optimal semi matching

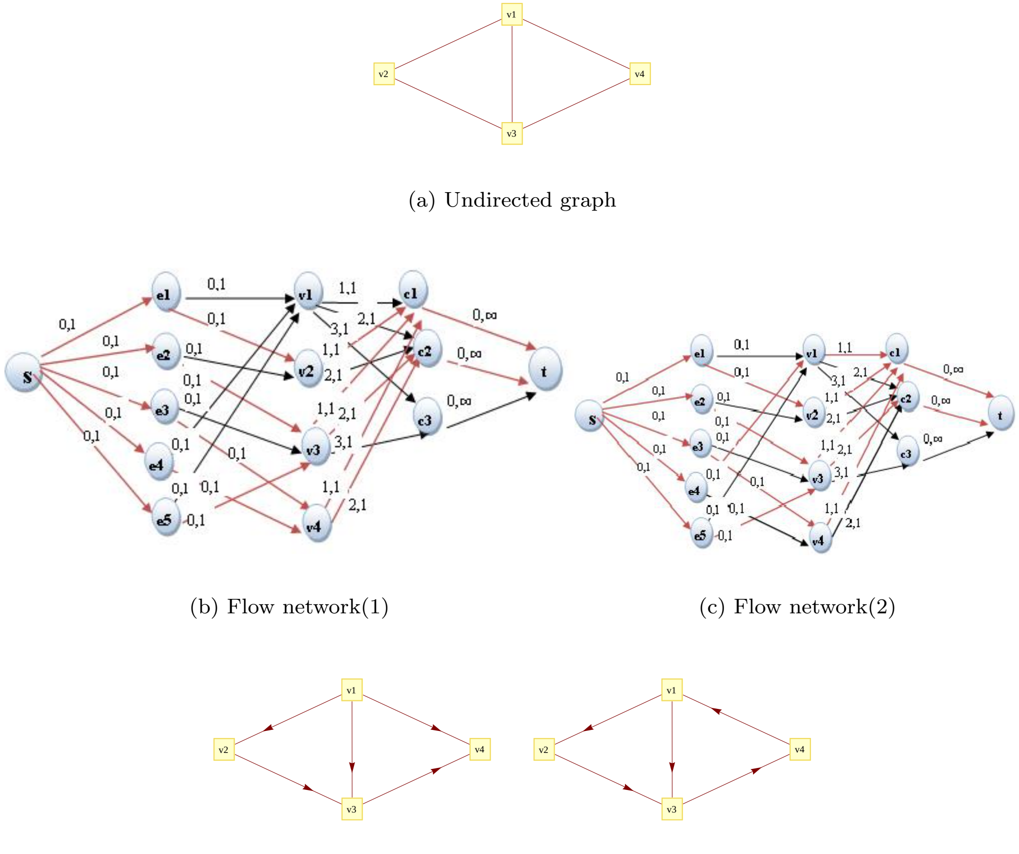
Figure 30: Cost reducing paths and semi matching.

Definition 5.12 (Network)
A flow network is a directed graph $G = (V(G), E(G))$ with source s and sink t, where edge $(u, v) \in E(G)$ has capacity $c(u, v) > 0$, flow $f(u, v) \geq 0$ and $cost(u, v) \geq 0$. For each $(u, v) \in E(G)$, $f(u, v) \leq c(u, v)$ and $\sum_u f(u, v) = \sum_u f(v, u)$.

Definition 5.13 (Maximum Flow)
The value of the flow is $\sum_{u \in V} f(s, u)$ and is the amount of the flow passing from the source to sink. Maximum flow is the maximum flow passing from source s to sink t. If the flow on the edge is equal to its capacity then the flow is called saturated.

Proposition 5.5 ([23])
Let $G_u = (V_u, E_u)$ be an undirected graph. Define a bipartite graph $G = (U, V, E)$ such that $U = E_u$, $V = V_u$ and $E = \{(u_1, v_1) \mid u_1 = (u, v) \in E_u, u = v_1 \text{ or } v = v_1\}$. Let $N = (V_N, E_N, C_N)$ be a network flow constructed from G such that $V_N = (U \cup V) \cup \{s\} \cup \{t\}$, $E_N = \{(s, u_i) \mid u_i \in U\} \cup \{(u_i, v_j) \mid u_i \in U, v_j \in V\} \cup \{(v_i, c_j) \mid 1 \leq i \leq |V|, 1 \leq j \leq d^{out}(i)\} \cup \{(c_i, t) \mid 1 \leq i \leq \triangle(G_u)\}$, where s and t denotes a source and a sink. The edges connecting s to u_i and u_i to v_j has cost 0 and capacity 1. Each vertex v_i connects to the cost centers with capacity 1 and cost $1, 2, \ldots, d^{out}(i)$ of G_u. If f is a maximum integral flow in N then f determines a semi-matching in G_u.

(Proof) Since all edges from s to U have a unit capacity, total capacity is $|U|$. If this cut has a maximum flow then each vertex carry one unit of flow from U to V. That is each vertex in the set U is matched with the vertex in V and the graph represent a semi matching M. Since the value of the maximum flow is equal to the capacity of the minimum cut and this cut is saturated in any flow, and then the flow in f induces the semi matching. ■



(a) Undirected graph

(b) Flow network(1)

(c) Flow network(2)

(d) Orientated graph(1)

(e) Oriented graph(2)

Figure 31: Network flow and semi matching.

Example 5.8
The Figure 31(a) shows an undirected graph and the Figure 31(b) and Figure 31(c) shows the network flow constructed for it. Oriented graphs in the Figure 31(d) and Figure 31(e) shows the orientations obtained from the network flow.

We can construct an optimal semi matching algorithm as in the Table 5.7.

Theorem 5.17
Let $G_u = (V_u, E_u)$ be an undirected graph and $G_d = (V_d, E_d) = OSM(G_u)$. Then $LE(G_d) = LE_{opt}(G_u)$.

■

Any directed graph $G_d = (V_d, E_d)$ can be represented as a bipartite graph $G = (U, V, E)$, where

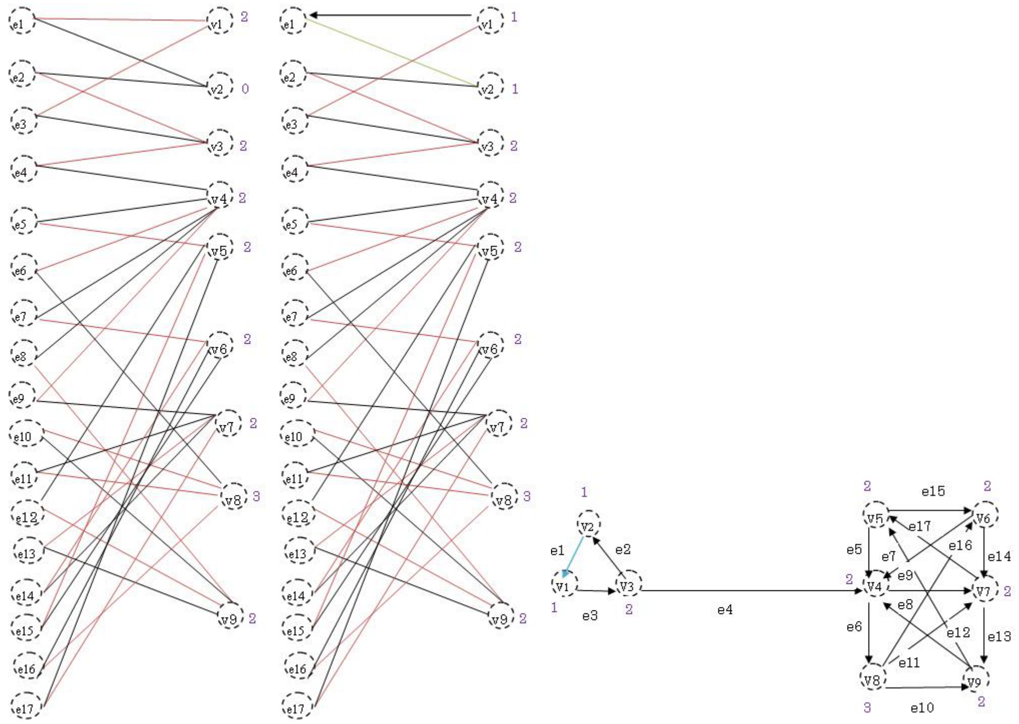
Input	An undirected graph $G_u = (V_u, E_u)$.
Output	An oriented graph $OSM(G_u) = G_d = (V_d, E_d)$.
Step 1:	Construct the bipartite graph $G_b = (U_b, V_b, E_b)$, where $U_b = E_u$, $V_b = V_u$ and $E_b = \{(u, v) \mid u = (v_1, v_2), (v_1, v) \in E_u\}$.
Step 2:	Assign an arbitrary semi matching M.
Step 3:	Let v_1 be $\max\{d_M(v) \vert v \in V_b\}$.
Step 4:	Find an alternate path $P = v_1 \to u_1 \to \cdots \to v_k$. of length $k(k \geq 1)$, which satisfy $d_M(v_i) \leq d_M(v_1)$ for $1 \leq i \leq k-1$ and $d_M(v_k) \leq d_M(v_1) - 2$. If such P exists then set $M = (M \setminus\ P) \cup \bar{P}$, where $\bar{P} = v_k \to \cdots \to v_1$ and goto Step 3. Otherwise halt.

Table 4: OSM algorithm.

$V = \{v \mid v \in V_d\}$ and $U = \{e \mid e \in E_d\}$. Then we can add two vertices, which is called source and sink to make a network flow. It is possible to find the optimal flow in the network and it is also possible to find the optimal oriented graph with minimum cost assign to vertices. However the order of the flow algorithms are $O(n+m)^3$. Here we consider MMO problem and apply it to minimize the maximum degree and obtain oriented graph. The order of the MMO algorithm introduced by [5] is $O(m^{1.5})$ and the one introduced by [45] is $O(m^2)$. The MMO which we consider here has a low order compare with flow algorithms.

As shown in the previous examples MMO not working properly on each graph. If MMO is failed then we can construct a bipartite graph for the resulted directed graph obtained from MMO, which has the minimum maximum outdegree. Then semi matching is optimal if there does not exists a cost reducing path by the Theorem 5.15. Lets consider the Figure 29 again. This can be represented as a bipartite graph $BG = (U_1, V_1, E_1)$ where $U_1 = E_d$ and $V_1 = V_d$ and $E_1 = \{(e_i, v_j), (e_i, v_k) \mid (v_j, v_k) \in V_d$ and $e_i \in E_d\}$ as in the Figure 32(a). Red lines indicate the semi-matching for the graph. Maximum outdegree is 3 and minimum outdegree is 0. There exists a cost reducing path $v_1 \to e_1 \to v_2$. By eliminating this cost reducing path, we obtain the graph as in the Figure 32(b), where green edge represent the arc add to semi matching. Optimal orientation obtained by removing cost reducing path is represented in the Figure 32(c).

Let $f(x) = \sum_{i=1}^{n} f(x_i)^2$, where $x_i \geq 0, f(x_i) = d^{out}(i)$ and there exists at least one i with $d^{out}(i) > 0$. Then $f''(x_i) = 2 > 0$ and $f(x_i)$ is a strictly convex function. Then $f(x) = \sum_{i=1}^{n}(d^{out}(i))^2$ is a strictly convex function. By the Theorem 5.16, semi-matching is optimal with respect to L_2 norm of its load vector. Hence the sum of squares of outdegrees of vertices and the resulted orientation has an optimal semi matching. By using MMO we can reduce the maximum outdegree and then by semi-matchings we can optimize the result by eliminating cost reducing paths. This yield the oriented graph with minimum Laplacian energy.



(a) Semi-matching (b) Optimal semi-matching (c) Optimal oriented graph

Figure 32: Optimal oriented graph using semi-matching.

5.8 Conclusion

We consider the problem of finding directed graphs with minimum Laplacian energy. First we derive a formula for Laplacian energy of directed graph using out degrees of vertices. Then we discuss the relationship between undirected and directed Laplacian energies. We enumerate the structure of directed graphs with Laplacian energy less than some integer value. Since we showed that Laplacian energy of a simple directed graph is the sum of squares of outdegrees, we can construct an algorithm to minimize the Laplacian energy of oriented graph by using semi matching algorithms.

6 Spectral clustering for directed graphs

6.1 Introduction

This chapter demonstrates experimental results of spectral clustering algorithms on directed graphs. Since a graph constructed by hyper links in web-pages is a directed graph, its adjacency matrix A is asymmetric and does not always have real eigenvalues. We extend undirected spectral clustering algorithms to the directed graphs using some transformation such as $A = A + A^T, A = AA^T$ and $A = A^T A$ and compare the resulted clusters. Then we apply the spectral clustering algorithms to directed graphs using the directed Laplacian introduced by Fan Chung [11] and k-means algorithms. We propose an algorithm which merge clusters by minimizing the normalized cut defined for directed graphs.

6.2 Spectral clustering on undirected graphs

This section explains the existing spectral clustering algorithms to find clusters in an undirected graph. We list three algorithms as listed in the Table 5, Table 6 and Table 7 using three kinds of Laplacian matrices. Number of clusters need to be decided in order to apply the algorithm. This number may or may not give optimal clustering results. If some one wants to find the optimal clusters then it is better to decide possible number of clusters in the graphs. There are several ways to get an idea of the appropriate number of clusters in a given graph. The following list some techniques useful to find the number of clusters.

1. **Eigengap heuristics and the eigenvectors:** *This can be used for any matrix. Here number of clusters k are chosen such that the first few eigenvalues $\lambda_1, \dots, \lambda_k$ are small and λ_{k+1} is relatively large. Similarly, the number of large gaps in the second eigenvector also gives an idea of number of clusters.*

2. **Modularity function:** *Modularity function Q is introduced in [39],[38] to find the association between groups. Q not only measure the quality of the particular division of the network but also useful to automatically select the optimal number of clusters by finding the cluster number which has a maximum Q value.*

3. **Commute distance:** *Measures the distance between vertices. Distance between the vertices to belong to same cluster is small and different clusters are large.*

Definition 6.1 (Modularity function)
Let $V_1, V_2, \dots, V_k$ are k clusters of the graph $G = (V(G), E(G))$. Then the modularity function $Q(k)$ of cluster k is defined as

$$Q(k) = \sum_{i=1}^{k} \left(\frac{w(V_i, V_i)}{w(V, V)} - \left(\frac{w(V_i, V)}{w(V, V)} \right)^2 \right),$$

where $w(V_i, V_i)$ measures the sum of edge weights withing the same cluster and $w(V_i, V)$ measures the sum of weights of edges between the vertices in V_i and all other vertices in V. We can write this much precisely as

$$Q(k) = \sum_{i=1}^{k} \left(\frac{vol(V_i)}{vol(G)} - \left(\frac{cut(V_i, V)}{vol(G)} \right)^2 \right).$$

Input	V a vertex set and E an edge set. k: number of clusters.
Step 1	Construct W weighted adjacency matrix with size $n \times n$.
Step 2	Find $L = D - W$.
Step 3	Find the first k eigenvectors $u_1, \dots, u_k$.
Step 4	Let $U \in \Re^{n \times k}$ be a matrix contain vectors $u_1, \dots, u_k$ as columns.
Step 5	Let $y_i \in \Re^k$ is a row vector of U for $i = 1, \dots, n$.
Step 6	Cluster points $(y_i)_{i=1,\dots,n} \in \Re^k$ with $k - means$ algorithm.
Step 7	Let clusters as C_i, $i = 1, \dots, k$.
Output	Clusters $A_1, \dots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Table 5: Clustering using difference Laplacian matrix.

Input	V a vertex set and E an edge set. k: number of clusters.
Step 1	Construct W weighted adjacency matrix with size $n \times n$.
Step 2	Find $\mathcal{L} = D^{-1/2} L D^{-1/2}$.
Step 3	Find the first k eigenvectors $u_1, \dots, u_k$.
Step 4	Let $U \in \Re^{n \times k}$ be a matrix contains the eigenvectors $u_1, \dots, u_k$ as columns.
Step 5	Form $U' = (u'_{ij})$ with size $n \times k$, where $u'_{ij} = u_{ij} / (\sum_k u_{ik}^2)^{1/2}$.
Step 5	Let $y_i \in \Re^k$ is a row vector of U' for $i = 1, \dots, n$.
Step 6	Cluster points $(y_i)_{i=1,\dots,n} \in \Re^k$ with $k - means$ algorithm.
Step 7	Let clusters as C_i, $i = 1, \dots, k$.
Output	Clusters $A_1, \dots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Table 6: Clustering using normalized Laplacian matrix.

k value respect to the maximum number of $Q(k)$ is the optimal number of clusters in the graph.

Definition 6.2 (Commute distance)
Commute distance for undirected weighted graph G is defined in [46] as $c_{ij} = vol(G)(l^*_{ii} - 2l^*_{ij} + l^*_{jj})$, where l^* is the generalized inverse of L. The matrix L can be decomposed as $L = ZRZ^T$, where Z is the matrix contains the eigenvectors as columns, R is the diagonal matrix with eigenvalues on diagonal. So the generalized inverse of L is defined as $l^* = ZR^*Z^T$, where

$$R^* = (r^*_{ij}) = \begin{cases} \frac{1}{\lambda_i}, & \text{if } \lambda_i \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Note. *We can replace the step 2 of the Table 5 by any matrix and apply the algorithm. Here we consider difference, normalized Laplacian matrix and Laplacian matrix L_{rw}.*

Input	V a vertex set and E an edge set. k: number of clusters.
Step 1	Construct W weighted adjacency matrix with size $n \times n$.
Step 2	Find $L = D - W$.
Step 3	Compute $L_{rw} = D^{-1}L$.
Step 4	Find the first k eigenvectors $u_1, \ldots, u_k$ of L_{rw}.
Step 5	Let $U \in \Re^{n \times k}$ be a matrix contains the eigenvectors $u_1, \ldots, u_k$ as columns.
Step 6	Let $y_i \in \Re^k$ is a row vector of U for $i = 1, \ldots, n$.
Step 7	Cluster points $(y_i)_{i=1,\ldots,n} \in \Re^k$ with $k - means$ algorithm.
Step 8	Let clusters as C_i, $i = 1, \ldots, k$.
Output	Clusters $A_1, \ldots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Table 7: Clustering using Laplacian matrix with random walk.

clus1	clus2	clus3	clus4
1	7	14	18
2	8	15	19
3	9	16	20
4	10	17	21
5	11		22
6	12		23
	13		

Table 8: Clusters obtained from the Figure 33(a).

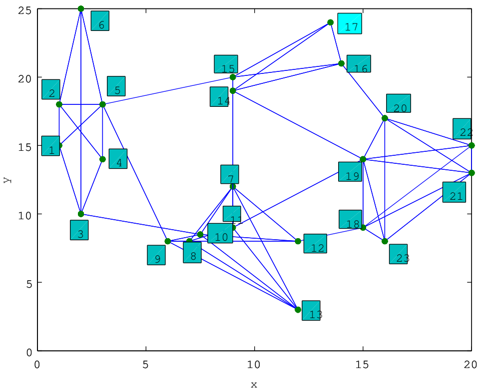
6.3 Experimental results

This section demonstrates experimental results on spectral clustering algorithms applied ton real world networks. Examples consider here are undirected.

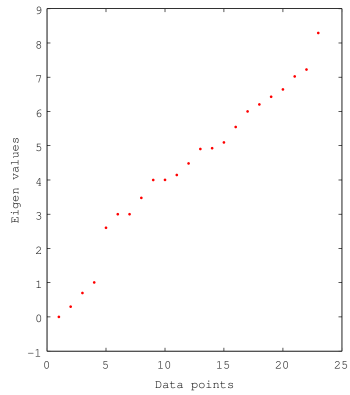
Example 6.1 (Find clusters in a small network graph)
Suppose we have a graph as in the Figure 33. We plot the difference Laplacian eigenvalues as in the Figure 33(b). First 4 eigenvalues are small and 5th eigenvalue is large. So by following eigengap heuristics, it is possible to have 4 clusters. The Figure 33(c) represent the second eigenvector. We can identify three considerable gaps between the second eigenvector values and this shows the existence of 4 clusters.

We use spectral clustering algorithm to find the clusters in the Figure 33(a) and we received 4 clusters as in the Table 8.

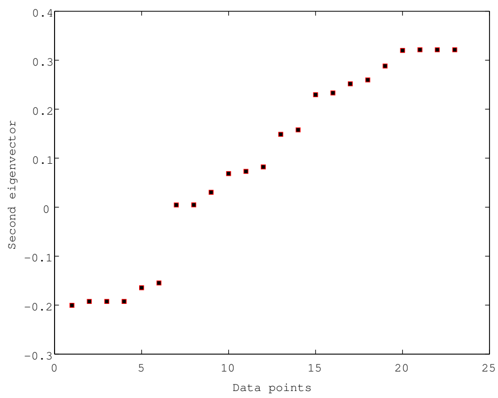
Example 6.2 (Find Q values)
We can merge the spectral clustering algorithms with the Q values. That is we can find the clusters and then calculate the Q values for each cluster number. Algorithm select the best number of clusters with respect to the maximum Q value. The Figure 34(a) shows



(a) Original data



(b) Eigenvalues of the difference Laplacian



(c) The second eigenvector

Figure 33: Identify the number of clusters using eigenvalues and the second eigenvector.

Q values for clusters generated by using $L, \mathcal{L}, L_{rw}$ for above Example 6.1. In the Figure 34(a), L is a difference Laplacian matrix, L_{sym} is a normalized Laplacian and L_{rw} is a difference Laplacian with random walk. The Figure 34(c) shows Q values obtained for the dolphin social network in the Figure 34(b) using normalized matrix. Data available at `http://www-personal.umich.edu/~mejn/netdata/`. *The Figure 34(d) shows Q values for football data. Data available at* `http://vlado.fmf.uni-i.si/pub/networks/data/sport/football.net`. *The Figure 34(c) shows 5 clusters with maximum Q value (0.4902), where [31] found 2 main communities and further divide into 4 sub communities. Q values between 0.3 and 0.7 shows a good relationship among the data. $Q < 0.3$ shows a weak relationship. We can select the best number of clusters by using the maximum value of Q.*

6.4 Random walk on directed graphs

Let $G = (V(G), E(G))$ be a directed graph with a vertex set $V(G)$ and an edge set $E(G)$. We denote the outdegree of vertex u as $d^{out}(u)$ and indegree as $d^{in}(u)$.

Definition 6.3 (Random walk)
A walk is a sequence of vertices $w = (v_0, v_1, \ldots, v_t)$ such that (v_i, v_{i+1}) is an edge. A random walk is defined by a transition probability matrix P, where $P(u, v)$ denotes the probability of moving from a vertex u to a vertex v.

Definition 6.4 (Transition probability matrix)
For a weighted directed graph with edge weights $w(u, v) > 0$ transition probability matrix P can be defined as

$$p(u,v) = \begin{cases} \frac{w_{uv}}{\sum_l (w_{ul})} & \text{if } (u,v) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

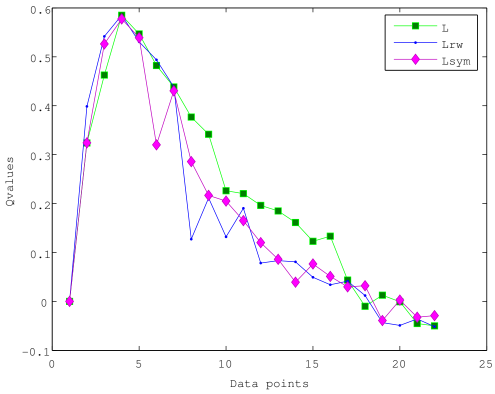
Clearly, $P(u, v) > 0$ only if $(u, v) \in E(G)$. Also,$\sum_v P(u, v) = 1$. However, for a directed graph, it is not required that $\sum_v P(u, v) = 1$ in general. According to the Perron-Frobenius theorem, transition probability matrix P of a strongly connected directed graph has a unique left eigenvector ϕ with $\phi(v) > 0$ for all v, and $\phi P = \phi$. The random walk on such a graph has a unique stationary distribution, which satisfy the balance equation $\phi(v) = \sum_{u \sim v} \phi(u)P(u, v)$ as well as $\sum_v \phi(v) = 1$. Generally, all directed graphs are not satisfy above condition. One possibility is to replace the random walk with teleporting random walk, which was used for page ranking in [40].

Definition 6.5 (Teleporting random walk)
Transition probability of this model can be written as follows.

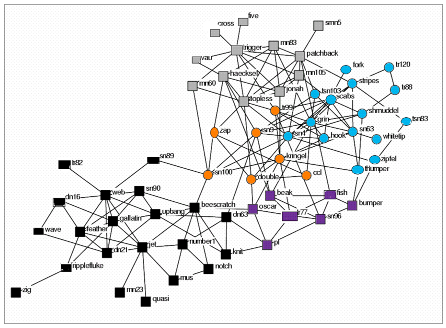
$$p_\varepsilon(u,v) = \begin{cases} \frac{1}{vol(G)} & \text{if } d^{out}(u) = 0, \\ \varepsilon * w_{u,v}/d^{out}(u) + (1-\varepsilon) * 1/vol(G) & \text{if } d^{out}(u) > 0. \end{cases}$$

Here ε is a damping factor $(0 < \varepsilon < 1)$ and $vol(G) = \sum_i (d^{out}(i) + d^{in}(i))$. Random walk move to next page by selecting a link with probability ε or it jumps to entire web with probability $(1 - \varepsilon)$.

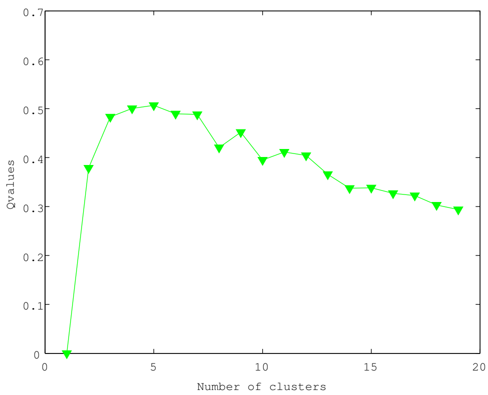
Definition 6.6 (Directed Laplacian Fan Chung [11])
The Laplacian L of a directed graph G is defined by $L = I - \dfrac{\psi^{1/2} P \psi^{-1/2} + \psi^{-1/2} P^t \psi^{1/2}}{2}$, where ψ is a diagonal matrix with entries $\psi(i, i) = \phi(i)$.



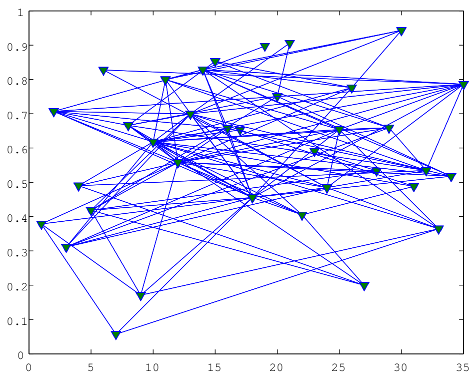
(a) Example 6.1



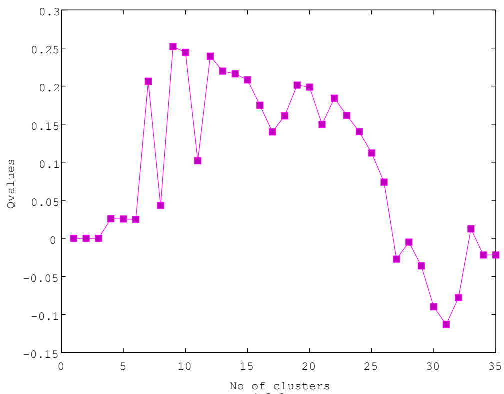
(b) Dolphin social network



(c) Q values of dolphin social network



(d) Football data - original graph



(e) Q values for football data

Figure 34: Q values for clusters.

Input	V a vertex set and E an edge set. k: number of clusters. P:transition probability matrix. ϕ: stationary distribution.
Step 1	Construct ψ with stationary distributions ϕ.
Step 2	Find $L = I - \frac{\psi^{1/2}P\psi^{-1/2}+\psi^{-1/2}P^t\psi^{1/2}}{2}$.
Step 3	Find the first k eigenvectors $u_1, \ldots, u_k$ of L.
Step 4	Let $U \in \Re^{n\times k}$ be a matrix contains the eigenvectors $u_1, \ldots, u_k$ as columns.
Step 5	Let $y_i \in \Re^k$ is a row vector of U for $i = 1, \ldots, n$.
Step 6	Cluster points $(y_i)_{i=1,\ldots,n} \in \Re^k$ with $k - means$ algorithm.
Step 7	Let clusters as C_i, $i = 1, \ldots, k$.
Output	Clusters $A_1, \ldots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Table 9: Clustering using directed Laplacian matrix.

Definition 6.7 (Out boundary)
Let $G = (V, E)$ be a directed graph. Let $S \subset G$. Then the out boundary of S is defined by $\partial S = \{(u, v) \in E(G) | u \in S, v \in V \setminus S\}$.

Definition 6.8 (Volume)
The volume of a subset $S \subset V(G)$ is denoted by $vol(S) = \sum_{v\in S} \phi(v)$ is the probability that the random walk occupies some vertex in S. Consequently $vol(V) = 1$. The volume of ∂S is denoted by $vol(\partial S) = \sum_{(u,v)\in\partial S} \phi(u)P(u, v)$ is the probability random walk jump from S to ∂S.

Definition 6.9 (Weighted Normalized Cut ($WNcut$))
Let S and $V \setminus S$ are disjoint sets in G. Let $\phi(i)$ be the stationary distribution. Then **WNcut** *for the directed graph can be defined as follows.*

$$\begin{aligned} WNcut(S, V \setminus S) &= \frac{cut(S, V \setminus S)}{vol(S)} + \frac{cut(V \setminus S, S)}{vol(V \setminus S)} \\ &= \frac{vol(\partial S)}{vol(S)} + \frac{vol(\partial(V \setminus S))}{vol(V \setminus S)} \end{aligned}$$

Since the probability which the random walk leaves a vertex is equal to the probability of arriving at a vertex, we have $vol(\partial S) = vol(\partial(V \setminus S))$. Then $WNcut(S, V \setminus S) = vol(\partial S)(\frac{1}{vol(S)} + \frac{1}{vol(V \setminus S)})$.

We can define the $WNcut(S_1, \ldots, S_n)$ for partitions $S_1, \ldots, S_n$ as $WNcut(S_1, \ldots, S_n) = \sum_{i=1}^{n} \frac{vol(\partial S_i)}{vol(S_i)}$. Good partition of a directed graph under this criteria corresponding to the cut such that probability of going from one community to another is small, while probability of remaining in the current cluster is high. Zhou et al.[50] find approximation to this minimization problem by solving the eigenvectors of the directed Laplacian. By following the above definitions, we can apply the clustering algorithm to a strongly connected directed graph. Our algorithm is given the Table 9.

If the graph is not a strongly connected directed graph then we can replace the random walk with teleporting random walk as defined above. Besides that there are some ways to extend the undirected spectral clusterings to directed clustering. We list some of methods here.

1. *Replace directed edges with undirected edges. This method directly transform directed graphs into undirected graphs and it also destroyed the valuable information on the edges.*

2. *Method of symmetrization. Since the adjacency matrix A of a directed graph is asymmetric, we can use the symmetric matrix $(A + A^T)/2$ instead of A. Then normalized Laplacian of the undirected graph changes to $\mathcal{L} = D^{-1/2}(D - \frac{(A+A^T)}{2})D^{-1/2}$. We can apply spectral clustering algorithms using this modified normalized Laplacian matrix.*

6.5 Comparison of clustering methods

Example 6.3
Graph given in the Figure 35(a) has directed and undirected edges. The Figure 35(b) is obtained by applying undirected spectral clustering methods. We have three clusters which consists of vertices $\{1, 2, 3, 4\}$,$\{10, 11, 12, 13\}$ and $\{5, 6, 7, 8, 9\}$. The Figure 35(c) is obtained by applying directed spectral clustering methods. There we obtained three clusters which consists of vertex $\{\{1, 2, 3, 4, 5\}, \{10, 11, 12, 13\}, \{6, 7, 8, 9\}\}$.

It is also interesting to compare the results of directed clustering methods and symmetrization transformations. The following example demonstrates different transformation methods.

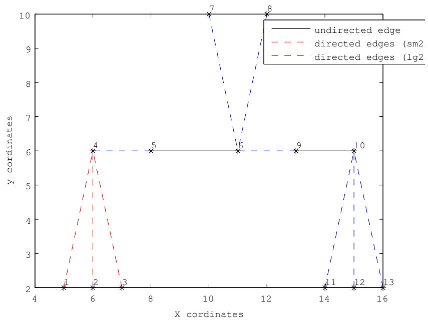
Example 6.4
We apply directed clustering method to find 2 clusters using teleporting random walk as in the Figure 36(d). Then we apply clustering with different transformations. According to the results, we obtained different clusters from different symmetrization methods as shown in the Figure 36(a), Figure 36(b) and Figure 36(c).

6.6 Proposed method by using merging techniques

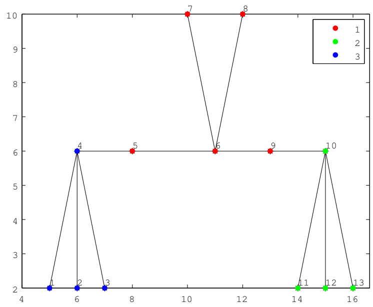
Suppose we need to find k clusters in the directed graph. By using directed spectral clustering method we can find $k' < k$ number of clusters initially. Then we merge two clusters by minimizing $WNcut$ value. Algorithm stop when we receive required number of clusters k. Here we demonstrates some example by applying this method.

Example 6.5
The Figure 37(a) show a directed graph with 2 known community structure. By observing the second eigenvector of directed Laplacian, we can identify the two partitions.

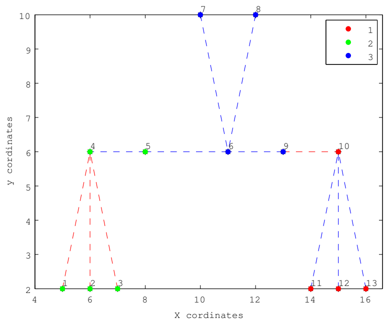
$$L = \begin{bmatrix} 1 & -.025 & -.25 & 0 & 0 & 0 & 0 \\ -.25 & 1 & -.075 & 0 & 0 & -.25 & 0 \\ -.25 & -.075 & 1 & -0.25 & -.25 & 0 & 0 \\ 0 & 0 & -.25 & 1 & -.025 & -0.25 & -0.5 \\ 0 & 0 & -.25 & -.025 & 1 & 0 & -0.25 \\ 0 & -.25 & 0 & -.025 & 0 & 1 & -0.25 \\ 0 & 0 & 0 & 1 & -0.5 & -0.25 & 1 \end{bmatrix},$$



(a) Network Graph



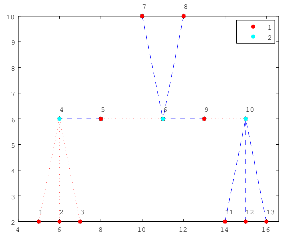
(b) Undirected clusters



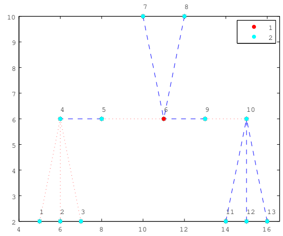
(c) Directed clusters

Figure 35: Directed and undirected clusters.

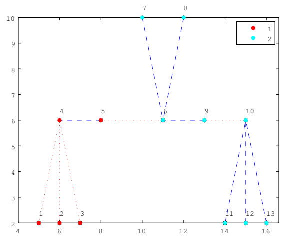
$$P = \begin{bmatrix} 0 & 0.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 & 0 & 0 & 0.5 \\ 0 & 0.5 & 0 & 0 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix},$$



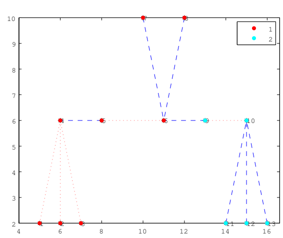
(a) Clusters using $A = A^T A$



(b) Clusters using $A = AA^T$



(c) Clusters using $A = (A + A^T)/2$



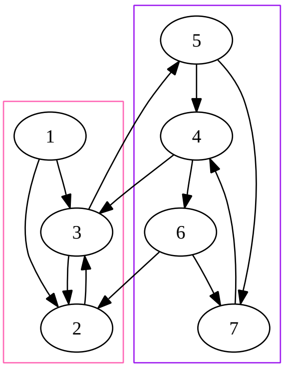
(d) Directed clustering

Figure 36: Clusters from directed and undirected clustering.

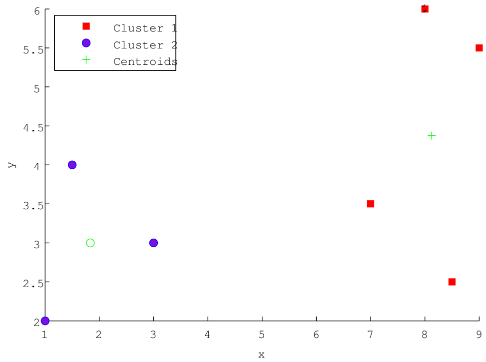
$$Y = \begin{bmatrix} 0.2372 & 0.3009 \\ 0.4913 & 0.4335 \\ 0.5462 & 0.3455 \\ 0.3928 & -0.4577 \\ 0.2850 & -0.2492 \\ 0.2724 & -0.2152 \\ 0.3071 & -0.5330 \end{bmatrix}.$$

Here L is the directed Laplacian matrix, P is the transition probability matrix and Y is the first two eigenvectors. By looking at the second eigenvector, it is clear that first 3 vertices are belong to one cluster. Since this graph is a strongly regular, we can easily apply spectral clustering algorithm and obtained two clusters as in the Figure 37(b).

Example 6.6
This example demonstrates our proposed method. First we find 7 clusters using directed spectral clustering methods. Then we apply merging techniques until we receive 2 clusters by minimizing $WNcut$ values. Resulted figures are listed in the Figure 38.



(a) Original graph



(b) Two Clusters

Figure 37: Directed graph with 2 clusters.

Even though the experimental results give good clustering results for small graphs, applying this method to large networks is computationally difficult since it need to consider several subsets and compute normalized cut in order to minimize the normalized cut. Other problems remained here are to find the stopping criteria, when we do not know the number of clusters we want to find. It is remained for the future to expand this algorithm to efficient one.

6.7 Conclusion

For the undirected graphs we have followed several clustering methods. We can apply Shi and Malik's [42] minimum normalized cut or spectral clustering algorithms to find clusters. But there is no way to select the best number of clusters. So it seemed that spectral clustering use with Newman modularity function performed well since it is possible to identify the best possible number of clusters. Here we use spectral algorithms to find the clusters in the directed Laplacian and use the multiple eigenvectors to find the k *clusters. We followed the techniques in [42] and proposed a merging algorithm for finding clusters in directed graphs. Our* $WNcut$ *definition is a generalization of [42], [11] and the one defined in [50]. The major disadvantage in our approach is applying the algorithm to a large network takes lot of memory to merging and minimizing normalized cut. It is remained for the future to improve the efficiency of the algorithm.*

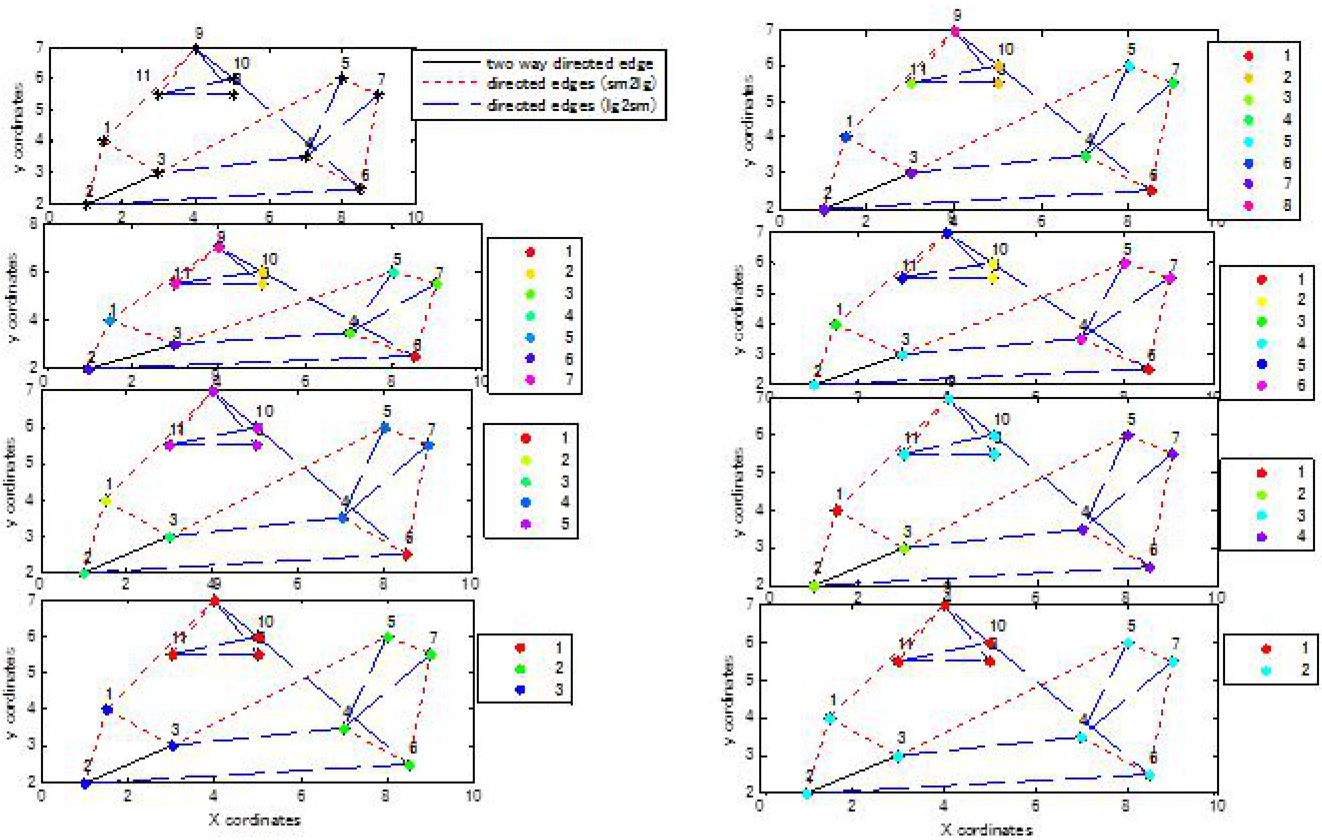


Figure 38: Clusters by merging method.

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