Spectral Theory of Unsigned and Signed Graphs Applications to Graph Clustering: a Survey

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Abstract: This is a survey of the method of graph cuts and its applications to graph clustering of weighted unsigned and signed graphs. I provide a fairly thorough treatment of the method of normalized graph cuts, a deeply original method due to Shi and Malik, including complete proofs. I also cover briefly the method of ratio cuts, and show how it can be viewed as a special case of normalized cuts. I include the necessary background on graphs and graph Laplacians. I then explain in detail how the eigenvectors of the graph Laplacian can be used to draw a graph. This is an attractive application of graph Laplacians. The main thrust of this paper is the method of normalized cuts. I give a detailed account for $K = 2$ clusters, and also for $K > 2$ clusters, based on the work of Yu and Shi. I also show how both graph drawing and normalized cut K-clustering can be easily generalized to handle signed graphs, which are weighted graphs in which the weight matrix W may have negative coefficients. Intuitively, negative coefficients indicate distance or dissimilarity. The solution is to replace the degree matrix D by the matrix $\overline{D}$ in which absolute values of the weights are used, and to replace the Laplacian $L = D - W$ by the signed Laplacian $\overline{L} = \overline{D} - W$. The signed Laplacian $\overline{L}$ is always positive semidefinite, and it may be positive definite (for unbalanced graphs, see Chapter 5). As far as I know, the generalization of K-way normalized clustering to signed graphs is new. Finally, I show how the method of ratio cuts, in which a cut is normalized by the size of the cluster rather than its volume, is just a special case of normalized cuts. All that needs to be done is to replace the normalized Laplacian L_{sym} by the unormalized Laplacian L. This is also true for signed graphs (where we replace $\overline{L}_{\mathrm{sym}}$ by $\overline{L}$).

Three points that do not appear to have been clearly articulated before are elaborated:

1. The solutions of the main optimization problem should be viewed as tuples in the K-fold cartesian product of projective space $\mathbb{RP}^{N-1}$.

2. When $K > 2$, the solutions of the relaxed problem should be viewed as elements of the Grassmannian $G(K, N)$.

3. Two possible Riemannian distances are available to compare the closeness of solutions: (a) The distance on $(\mathbb{RP}^{N-1})^K$. (b) The distance on the Grassmannian.

I also clarify what should be the necessary and sufficient conditions for a matrix to represent a partition of the vertices of a graph to be clustered.

Contents

Chapter 1

Introduction

In the Fall of 2012, my friend Kurt Reillag suggested that I should be ashamed about knowing so little about graph Laplacians and normalized graph cuts. These notes are the result of my efforts to rectify this situation.

I begin with a review of basic notions of graph theory. Even though the graph Laplacian is fundamentally associated with an undirected graph, I review the definition of both directed and undirected graphs. For both directed and undirected graphs, I define the degree matrix D, the incidence matrix B, and the adjacency matrix A. Then, I define a *weighted graph*. This is a pair (V, W), where V is a finite set of nodes and W is a $m \times m$ symmetric matrix with nonnegative entries and zero diagonal entries (where $m = |V|$). For every node $v_i \in V$, the *degree* $d(v_i)$ (or d_i) of v_i is the sum of the weights of the edges adjacent to v_i:

$$d_i = d(v_i) = \sum_{j=1}^{m} w_{ij}.$$

The *degree matrix* is the diagonal matrix

$$D = \mathrm{diag}(d_1, \ldots, d_m).$$

Given any subset of nodes $A \subseteq V$, we define the *volume* $\mathrm{vol}(A)$ of A as the sum of the weights of all edges adjacent to nodes in A:

$$\mathrm{vol}(A) = \sum_{v_i \in A} \sum_{j=1}^{m} w_{ij}.$$

The notions of degree and volume are illustrated in Figure 1.1. Given any two subsets $A, B \subseteq V$ (not necessarily distinct), we define $\mathrm{links}(A, B)$ by

$$\mathrm{links}(A, B) = \sum_{v_i \in A, v_j \in B} w_{ij}.$$

The quantity $\text{links}(A, \overline{A}) = \text{links}(\overline{A}, A)$ (where $\overline{A} = V - A$ denotes the complement of A in V) measures how many links escape from A (and $\overline{A}$). We define the *cut* of A as

$$\text{cut}(A) = \text{links}(A, \overline{A}).$$

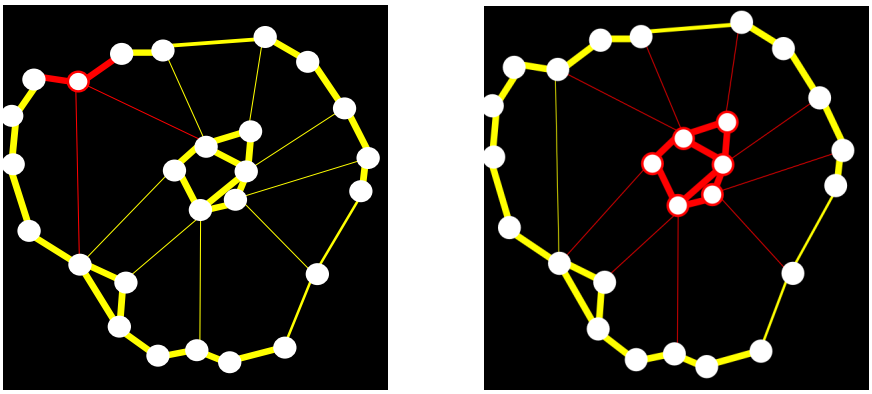

Figure 1.1: Degree and volume.

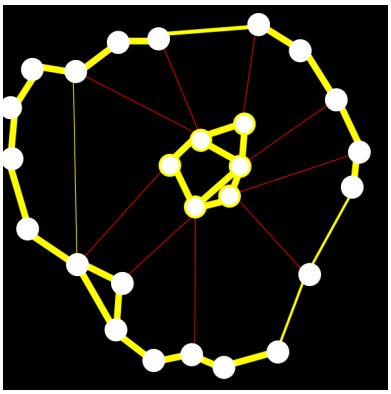

Figure 1.2: A Cut involving the set of nodes in the center and the nodes on the perimeter.

The notions of cut is illustrated in Figure 1.2. The above concepts play a crucial role in the theory of normalized cuts. Then, I introduce the (unnormalized) *graph Laplacian* L of a directed graph G in an "old-fashion," by showing that for any orientation of a graph G,

$$BB^\top = D - A = L$$

is an invariant. I also define the (unnormalized) *graph Laplacian* L of a weighted graph $G = (V, W)$ as $L = D - W$. I show that the notion of incidence matrix can be generalized

to weighted graphs in a simple way. For any graph G^σ obtained by orienting the underlying graph of a weighted graph $G = (V, W)$, there is an incidence matrix B^σ such that

$$B^\sigma (B^\sigma)^\top = D - W = L.$$

I also prove that

$$x^\top L x = \frac{1}{2} \sum_{i,j=1}^{m} w_{i\,j} (x_i - x_j)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

Consequently, $x^\top L x$ does not depend on the diagonal entries in W, and if $w_{i\,j} \geq 0$ for all $i, j \in \{1, \ldots, m\}$, then L is positive semidefinite. Then, if W consists of nonnegative entries, the eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_m$ of L are real and nonnegative, and there is an orthonormal basis of eigenvectors of L. I show that the number of connected components of the graph $G = (V, W)$ is equal to the dimension of the kernel of L, which is also equal to the dimension of the kernel of the transpose $(B^\sigma)^\top$ of any incidence matrix B^σ obtained by orienting the underlying graph of G.

I also define the normalized graph Laplacians L_{sym} and L_{rw}, given by

$$\begin{aligned} L_{\text{sym}} &= D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2} \\ L_{\text{rw}} &= D^{-1} L = I - D^{-1} W, \end{aligned}$$

and prove some simple properties relating the eigenvalues and the eigenvectors of L, L_{sym} and L_{rw}. These normalized graph Laplacians show up when dealing with normalized cuts.

Next, I turn to *graph drawings* (Chapter 3). Graph drawing is a very attractive application of so-called spectral techniques, which is a fancy way of saying that that eigenvalues and eigenvectors of the graph Laplacian are used. Furthermore, it turns out that graph clustering using normalized cuts can be cast as a certain type of graph drawing.

Given an undirected graph $G = (V, E)$, with $|V| = m$, we would like to draw G in $\mathbb{R}^n$ for n (much) smaller than m. The idea is to assign a point $\rho(v_i)$ in $\mathbb{R}^n$ to the vertex $v_i \in V$, for every $v_i \in V$, and to draw a line segment between the points $\rho(v_i)$ and $\rho(v_j)$. Thus, a *graph drawing* is a function $\rho \colon V \to \mathbb{R}^n$.

We define the *matrix of a graph drawing ρ (in $\mathbb{R}^n$)* as a $m \times n$ matrix R whose ith row consists of the row vector $\rho(v_i)$ corresponding to the point representing v_i in $\mathbb{R}^n$. Typically, we want $n < m$; in fact n should be much smaller than m.

Since there are infinitely many graph drawings, it is desirable to have some criterion to decide which graph is better than another. Inspired by a physical model in which the edges are springs, it is natural to consider a representation to be better if it requires the springs to be less extended. We can formalize this by defining the *energy* of a drawing R by

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} \left\| \rho(v_i) - \rho(v_j) \right\|^2,$$

where $\rho(v_i)$ is the ith row of R and $\|\rho(v_i) - \rho(v_j)\|^2$ is the square of the Euclidean length of the line segment joining $\rho(v_i)$ and $\rho(v_j)$.

Then, "good drawings" are drawings that minimize the energy function $\mathcal{E}$. Of course, the trivial representation corresponding to the zero matrix is optimum, so we need to impose extra constraints to rule out the trivial solution.

We can consider the more general situation where the springs are not necessarily identical. This can be modeled by a symmetric weight (or stiffness) matrix $W = (w_{ij})$, with $w_{ij} \geq 0$. In this case, our energy function becomes

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} w_{ij} \|\rho(v_i) - \rho(v_j)\|^2 .$$

Following Godsil and Royle [10], we prove that

$$\mathcal{E}(R) = \mathrm{tr}(R^\top L R),$$

where

$$L = D - W,$$

is the familiar unnormalized Laplacian matrix associated with W, and where D is the degree matrix associated with W.

It can be shown that there is no loss in generality in assuming that the columns of R are pairwise orthogonal and that they have unit length. Such a matrix satisfies the equation $R^\top R = I$ and the corresponding drawing is called an *orthogonal drawing*. This condition also rules out trivial drawings.

Then, I prove the main theorem about graph drawings (Theorem 3.2), which essentially says that the matrix R of the desired graph drawing is constituted by the n eigenvectors of L associated with the smallest nonzero n eigenvalues of L. We give a number examples of graph drawings, many of which are borrowed or adapted from Spielman [21].

The next chapter (Chapter 4) contains the "meat" of this document. This chapter is devoted to the method of normalized graph cuts for graph clustering. This beautiful and deeply original method first published in Shi and Malik [20], has now come to be a "textbook chapter" of computer vision and machine learning. It was invented by Jianbo Shi and Jitendra Malik, and was the main topic of Shi's dissertation. This method was extended to $K \geq 3$ clusters by Stella Yu in her dissertation [23], and is also the subject of Yu and Shi [24].

Given a set of data, the goal of clustering is to partition the data into different groups according to their similarities. When the data is given in terms of a similarity graph G, where the weight $w_{i\,j}$ between two nodes v_i and v_j is a measure of similarity of v_i and v_j, the problem can be stated as follows: Find a partition $(A_1, \ldots, A_K)$ of the set of nodes V into different groups such that the edges between different groups have very low weight (which

indicates that the points in different clusters are dissimilar), and the edges within a group have high weight (which indicates that points within the same cluster are similar).

The above graph clustering problem can be formalized as an optimization problem, using the notion of cut mentioned earlier. If we want to partition V into K clusters, we can do so by finding a partition $(A_1, \ldots, A_K)$ that minimizes the quantity

$$\mathrm{cut}(A_1, \ldots, A_K) = \frac{1}{2} \sum_{i=1}^{K} \mathrm{cut}(A_i) = \frac{1}{2} \sum_{i=1}^{K} \mathrm{links}(A_i, \overline{A}_i).$$

For $K = 2$, the mincut problem is a classical problem that can be solved efficiently, but in practice, it does not yield satisfactory partitions. Indeed, in many cases, the mincut solution separates one vertex from the rest of the graph. What we need is to design our cost function in such a way that it keeps the subsets A_i "reasonably large" (reasonably balanced).

An example of a weighted graph and a partition of its nodes into two clusters is shown in Figure 1.3.

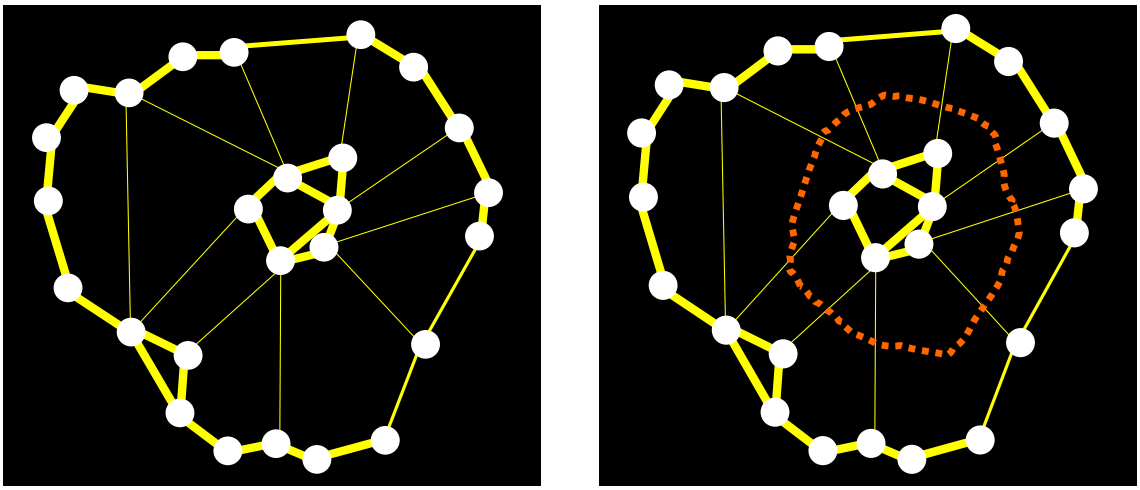

Figure 1.3: A weighted graph and its partition into two clusters.

A way to get around this problem is to normalize the cuts by dividing by some measure of each subset A_i. A solution using the volume $\mathrm{vol}(A_i)$ of A_i (for $K = 2$) was proposed and investigated in a seminal paper of Shi and Malik [20]. Subsequently, Yu (in her dissertation [23]) and Yu and Shi [24] extended the method to $K > 2$ clusters. The idea is to minimize the cost function

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{links}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)} = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)}.$$

The first step is to express our optimization problem in matrix form. In the case of two clusters, a single vector Xx can be used to describe the partition $(A_1, A_2) = (A, \overline{A})$. We need to choose the structure of this vector in such a way that

$$\mathrm{Ncut}(A, \overline{A}) = \frac{X^\top LX}{X^\top DX},$$

where the term on the right-hand side is a Rayleigh ratio.

After careful study of the original papers, I discovered various facts that were implicit in these works, but I feel are important to be pointed out explicitly.

First, I realized that it is important to pick a vector representation which is invariant under multiplication by a nonzero scalar, because the Rayleigh ratio is scale-invariant, and it is crucial to take advantage of this fact to make the denominator go away. This implies that *the solutions X are points in the projective space $\mathbb{RP}^{N-1}$*. This was my first revelation.

Let $N = |V|$ be the number of nodes in the graph G. In view of the desire for a scale-invariant representation, it is natural to assume that the vector X is of the form

$$X = (x_1, \ldots, x_N),$$

where $x_i \in \{a, b\}$ for $i = 1, \ldots, N$, for any two distinct real numbers a, b. This is an indicator vector in the sense that, for $i = 1, \ldots, N$,

$$x_i = \begin{cases} a & \text{if } v_i \in A \\ b & \text{if } v_i \notin A. \end{cases}$$

The choice $a = +1, b = -1$ is natural, but premature. The correct interpretation is really to view X as a representative of a point in the real projective space $\mathbb{RP}^{N-1}$, namely the point $\mathbb{P}(X)$ of homogeneous coordinates $(x_1 \colon \cdots \colon x_N)$.

Let $d = \mathbf{1}^\top D\mathbf{1}$ and $\alpha = \mathrm{vol}(A)$, where $\mathbf{1}$ denotes the vector whose components are all equal to 1. I prove that

$$\mathrm{Ncut}(A, \overline{A}) = \frac{X^\top LX}{X^\top DX}$$

holds iff the following condition holds:

$$a\alpha + b(d - \alpha) = 0. \tag{$\dagger$}$$

Note that condition ($\dagger$) applied to a vector X whose components are a or b is equivalent to the fact that X is orthogonal to $D\mathbf{1}$, since

$$X^\top D\mathbf{1} = \alpha a + (d - \alpha)b,$$

where $\alpha = \mathrm{vol}(\{v_i \in V \mid x_i = a\})$.

If we let

$$\mathcal{X} = \big\{(x_1, \ldots, x_N) \mid x_i \in \{a, b\},\ a, b \in \mathbb{R},\ a, b \neq 0\big\},$$

our solution set is

$$\mathcal{K} = \big\{X \in \mathcal{X} \mid X^\top D\mathbf{1} = 0\big\}.$$

Actually, to be perfectly rigorous, we are looking for solutions in $\mathbb{RP}^{N-1}$, so our solution set is really

$$\mathbb{P}(\mathcal{K}) = \big\{(x_1 \colon \cdots \colon x_N) \in \mathbb{RP}^{N-1} \mid (x_1, \ldots, x_N) \in \mathcal{K}\big\}.$$

Consequently, our minimization problem can be stated as follows:

Problem PNC1

$$\begin{array}{lll} \text{minimize} & \dfrac{X^\top LX}{X^\top DX} & \\ \text{subject to} & X^\top D\mathbf{1} = 0, & X \in \mathcal{X}. \end{array}$$

It is understood that the solutions are points $\mathbb{P}(X)$ in $\mathbb{RP}^{N-1}$.

Since the Rayleigh ratio and the constraints $X^\top D\mathbf{1} = 0$ and $X \in \mathcal{X}$ are scale-invariant, we are led to the following formulation of our problem:

Problem PNC2

$$\begin{array}{llll} \text{minimize} & X^\top LX & & \\ \text{subject to} & X^\top DX = 1, & X^\top D\mathbf{1} = 0, & X \in \mathcal{X}. \end{array}$$

Because problem PNC2 requires the constraint $X^\top DX = 1$ to be satisfied, it does not have the same set of solutions as problem PNC1 , but PNC2 and PNC1 are equivalent in the sense that they have the same set of minimal solutions as points $\mathbb{P}(X) \in \mathbb{RP}^{N-1}$ given by their homogeneous coordinates X. More precisely, if X is any minimal solution of PNC1, then $X/(X^\top DX)^{1/2}$ is a minimal solution of PNC2 (with the same minimal value for the objective functions), and if X is a minimal solution of PNC2, then λX is a minimal solution for PNC1 for all $\lambda \neq 0$ (with the same minimal value for the objective functions).

Now, as in the classical papers, we consider the relaxation of the above problem obtained by dropping the condition that $X \in \mathcal{X}$, and proceed as usual. However, having found a solution Z to the relaxed problem, we need to find a discrete solution X such that $d(X, Z)$ is minimum in $\mathbb{RP}^{N-1}$. All this is presented in Section 4.2.

If the number of clusters K is at least 3, then we need to choose a matrix representation for partitions on the set of vertices. It is important that such a representation be scale-invariant, and it is also necessary to state necessary and sufficient conditions for such matrices to represent a partition (to the best of our knowledge, these points are not clearly articulated in the literature).

We describe a partition $(A_1, \ldots, A_K)$ of the set of nodes V by an $N \times K$ matrix $X = [X^1 \cdots X^K]$ whose columns $X^1, \ldots, X^K$ are indicator vectors of the partition $(A_1, \ldots, A_K)$. Inspired by what we did when $K = 2$, we assume that the vector X^j is of the form

$$X^j = (x_1^j, \ldots, x_N^j),$$

where $x_i^j \in \{a_j, b_j\}$ for $j = 1, \ldots, K$ and $i = 1, \ldots, N$, and where a_j, b_j are any two distinct real numbers. The vector X^j is an indicator vector for A_j in the sense that, for $i = 1, \ldots, N$,

$$x_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ b_j & \text{if } v_i \notin A_j. \end{cases}$$

The choice $\{a_j, b_j\} = \{0, 1\}$ for $j = 1, \ldots, K$ is natural, but premature. I show that if we pick $b_i = 0$, then we have

$$\frac{\text{cut}(A_j, \overline{A_j})}{\text{vol}(A_j)} = \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \quad j = 1, \ldots, K,$$

which implies that

$$\text{Ncut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\text{cut}(A_j, \overline{A_j})}{\text{vol}(A_j)} = \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j}.$$

Then, I give necessary and sufficient conditions for a matrix X to represent a partition.

If we let

$$\mathcal{X} = \Big\{ [X^1 \ \ldots \ X^K] \mid X^j = a_j(x_1^j, \ldots, x_N^j),\ x_i^j \in \{1, 0\}, a_j \in \mathbb{R},\ X^j \neq 0 \Big\}$$

(note that the condition $X^j \neq 0$ implies that $a_j \neq 0$), then the set of matrices representing partitions of V into K blocks is

$$\begin{aligned} \mathcal{K} = \Big\{ X = [X^1 \cdots X^K] \quad \mid \quad & X \in \mathcal{X}, \\ & (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1} \Big\}. \end{aligned}$$

As in the case $K = 2$, to be rigorous, the *solution are really K-tuples of points in* $\mathbb{RP}^{N-1}$, so our solution set is really

$$\mathbb{P}(\mathcal{K}) = \Big\{ (\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)) \mid [X^1 \cdots X^K] \in \mathcal{K} \Big\}.$$

Remark: For any $X \in \mathcal{X}$, the condition $X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}$ is redundant. However, when we relax the problem and drop the condition $X \in \mathcal{X}$, the condition $X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}$ captures the fact $\mathbf{1}$ should be in the range of X.

In view of the above, we have our first formulation of K-way clustering of a graph using normalized cuts, called problem PNC1 (the notation PNCX is used in Yu [23], Section 2.1):

K-way Clustering of a graph using Normalized Cut, Version 1: Problem PNC1

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \\ \text{subject to} & (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}, \qquad\qquad X \in \mathcal{X}. \end{array}$$

As in the case $K = 2$, the solutions that we are seeking are K-tuples $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K))$ of points in $\mathbb{RP}^{N-1}$ determined by their homogeneous coordinates $X^1, \ldots, X^K$.

Then, step by step, we transform problem PNC1 into an equivalent problem PNC2. We eventually relax PNC1 into $(*_1)$ and PNC2 into $(*_2)$, by dropping the condition that $X \in \mathcal{X}$.

Our second revelation is that the relaxation $(*_2)$ of version 2 of our minimization problem (PNC2), which is equivalent to version 1, reveals that that the solutions of the relaxed problem $(*_2)$ are members of the *Grassmannian* $G(K, N)$.

This leads us to our third revelation: *we have two choices of metrics to compare solutions*: (1) a metric on $(\mathbb{RP}^{N-1})^K$; (2) a metric on $G(K, N)$. We discuss the first choice, which is the choice implicitly adopted by Shi and Yu. However, in approximating a discrete solution X by a solution Z of problem $(*_1)$ we allow more general transformations of the form $Q = R\Lambda$, where $R \in \mathbf{O}(K)$, and Λ is a diagonal invertible matrix. Thus we seek R and Λ to minimize $\|X - ZR\Lambda\|_F$. This yields better discrete solutions X.

In Chapter 5, I show how both the spectral method for graph drawing and the normalized-cut method for K clusters generalize to signed graphs, which are graphs whose weight matrix W may contain negative entries. The intuition is that negative weights indicate dissimilarity or distance.

The first obstacle is that the degree matrix may now contain negative entries. As a consequence, the Laplacian L may no longer be positive semidefinite, and worse, $D^{-1/2}$ may not exist.

A simple remedy is to use the absolute values of the weights in the degree matrix! We denote this matrix by $\overline{D}$, and define the *signed Laplacian* as $\overline{L} = \overline{D} - W$. The idea to use positive degrees of nodes in the degree matrix of a signed graph with weights $(-1, 0, 1)$ occurs in Hou [14]. The natural step of using absolute values of weights in the degree matrix is taken by Kolluri, Shewchuk and O'Brien [15] and Kunegis et al. [16].

As we will see, this trick allows the whole machinery that we have presented to be used to attack the problem of clustering signed graphs using normalized cuts.

As in the case of unsigned weighted graphs, for any orientation G^σ of the underlying graph of a signed graph $G = (V, W)$, there is an incidence matrix B^σ such that

$$B^\sigma (B^\sigma)^\top = \overline{D} - W = \overline{L}.$$

Consequently, $B^\sigma (B^\sigma)^\top$ is independent of the orientation of the underlying graph of G and $\overline{L} = \overline{D} - W$ is symmetric and positive semidefinite. I also show that

$$x^\top \overline{L} x = \frac{1}{2} \sum_{i,j=1}^{m} |w_{ij}|(x_i - \mathrm{sgn}(w_{ij}) x_j)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

As in Section 4.3, given a partition of V into K clusters $(A_1, \ldots, A_K)$, if we represent the jth block of this partition by a vector X^j such that

$$X_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ 0 & \text{if } v_i \notin A_j, \end{cases}$$

for some $a_j \neq 0$, then the following result holds: For any vector X^j representing the jth block of a partition $(A_1, \ldots, A_K)$ of V, we have

$$(X^j)^\top \overline{L} X^j = a_j^2 (\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)).$$

The above suggests defining the key notion of signed normalized cut: The *signed normalized cut* $\mathrm{sNcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ is defined as

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)} + 2 \sum_{j=1}^{K} \frac{\mathrm{links}^-(A_j, A_j)}{\mathrm{vol}(A_j)}.$$

Our definition of a signed normalized cut appears to be novel.

Based on previous computations, we have

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j},$$

where X is the $N \times K$ matrix whose jth column is X^j.

Observe that minimizing $\mathrm{sNcut}(A_1, \ldots, A_K)$ amounts to minimizing the number of positive and negative edges between clusters, and also minimizing the number of negative edges within clusters. This second minimization captures the intuition that nodes connected by a negative edge should not be together (they do not "like" each other; they should be far from each other). It would be preferable if the notion of signed cut only took into account the contribution $\mathrm{links}^+(A_j, \overline{A_j})$ of the positively weighted edges between disjoint clusters, but we have not found a way to achieve this.

Since

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j},$$

the whole machinery of Sections 4.3 and 4.5 can be applied with D replaced by $\overline{D}$ and L replaced by $\overline{L}$. However, there is a new phenomenon, which is that $\overline{L}$ may be positive definite. As a consequence, $\mathbf{1}$ is not always an eigenvector of $\overline{L}$.

Following Kunegis et al. [16], we show that the signed Laplacian $\overline{L}$ is positive definite iff G is unbalanced, which means that it contains some cycle with an odd number of negative edges. We also characterize when a graph is balanced in terms of the kernel of the transpose $B^\top$ of any of its incidence matrices.

To generalize the graph drawing method to signed graphs, we explain that if the energy function $\mathcal{E}(R)$ of a graph drawing is redefined to be

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} |w_{ij}| \left\| \rho(v_i) - \mathrm{sgn}(w_{ij}) \rho(v_j) \right\|^2,$$

then we obtain orthogonal graph drawings of minimal energy, and we give some examples.

We conclude this survey with a short chapter on graph clustering using ratio cuts. The idea of ratio cut is to replace the volume $\mathrm{vol}(A_j)$ of each block A_j of the partition by its size, $|A_j|$ (the number of nodes in A_j). Given an unsigned graph (V, W), the *ratio cut* $\mathrm{Rcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ is defined as

$$\mathrm{Rcut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{|A_j|}.$$

If we represent the jth block of this partition by a vector X^j such that

$$X_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ 0 & \text{if } v_i \notin A_j, \end{cases}$$

for some $a_j \neq 0$, then we obtain

$$\mathrm{Rcut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{|A_j|} = \sum_{i=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top X^j}.$$

On the other hand, the normalized cut is given by

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{\mathrm{vol}(A_j)} = \sum_{i=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j}.$$

Therefore, ratio cut is the special case of normalized cut where $D = I$! Consequently, all that needs to be done is to replace the normalized Laplacian L_{sym} by the unormalized Laplacian L (and omit the step of considering Problem $(**_1)$).

In the case of signed graphs, we define the *signed ratio cut* $\mathrm{sRcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ as

$$\mathrm{sRcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{|A_j|} + 2 \sum_{j=1}^{K} \frac{\mathrm{links}^-(A_j, A_j)}{|A_j|}.$$

Since we still have

$$(X^j)^\top \overline{L} X^j = a_j^2(\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)),$$

we obtain

$$\mathrm{sRcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top X^j}.$$

Therefore, this is similar to the case of unsigned graphs, with L replaced with $\overline{L}$. The same algorithm applies, but as in Chapter 5, the signed Laplacian $\overline{L}$ is positive definite iff G is unbalanced.

Some of the most technical material on the Rayleigh ratio, which is needed for some proofs in Chapter 3, is the object of Appendix A. Appendix B may seem a bit out of place. Its purpose is to explain how to define a metric on the projective space $\mathbb{RP}^n$. For this, we need to review a few notions of differential geometry.

I hope that these notes will make it easier for people to become familiar with the wonderful theory of normalized graph cuts. As far as I know, except for a short section in one of Gilbert Strang's book, and von Luxburg [22] excellent survey on spectral clustering, there is no comprehensive writing on the topic of graph cuts.

Chapter 2

Graphs and Graph Laplacians; Basic Facts

2.1 Directed Graphs, Undirected Graphs, Incidence Matrices, Adjacency Matrices, Weighted Graphs

Definition 2.1. A *directed graph* is a pair $G = (V, E)$, where $V = \{v_1, \ldots, v_m\}$ is a set of *nodes* or *vertices*, and $E \subseteq V \times V$ is a set of ordered pairs of distinct nodes (that is, pairs $(u, v) \in V \times V$ with $u \neq v$), called *edges*. Given any edge $e = (u, v)$, we let $s(e) = u$ be the *source* of e and $t(e) = v$ be the *target* of e.

Remark: Since an edge is a pair (u, v) with $u \neq v$, self-loops are not allowed. Also, there is at most one edge from a node u to a node v. Such graphs are sometimes called *simple graphs*.

An example of a directed graph is shown in Figure 2.1.

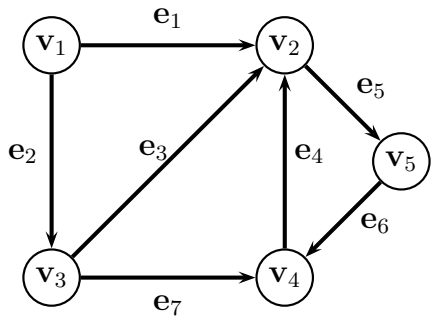

Figure 2.1: Graph G_1.

For every node $v \in V$, the *degree* $d(v)$ of v is the number of edges leaving or entering v:

$$d(v) = |\{u \in V \mid (v,u) \in E \text{ or } (u,v) \in E\}|.$$

We abbreviate $d(v_i)$ as d_i. The *degree matrix* $D(G)$, is the diagonal matrix

$$D(G) = \mathrm{diag}(d_1, \ldots, d_m).$$

For example, for graph G_1, we have

$$D(G_1) = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}.$$

Unless confusion arises, we write D instead of $D(G)$.

Definition 2.2. Given a directed graph $G = (V, E)$, for any two nodes $u, v \in V$, a *path from u to v* is a sequence of nodes $(v_0, v_1, \ldots, v_k)$ such that $v_0 = u$, $v_k = v$, and (v_i, v_{i+1}) is an edge in E for all i with $0 \leq i \leq k-1$. The integer k is the *length* of the path. A path is *closed* if $u = v$. The graph G is *strongly connected* if for any two distinct nodes $u, v \in V$, there is a path from u to v and there is a path from v to u.

Remark: The terminology *walk* is often used instead of *path*, the word path being reserved to the case where the nodes v_i are all distinct, except that $v_0 = v_k$ when the path is closed.

The binary relation on $V \times V$ defined so that u and v are related iff there is a path from u to v and there is a path from v to u is an equivalence relation whose equivalence classes are called the *strongly connected components* of G.

Definition 2.3. Given a directed graph $G = (V, E)$, with $V = \{v_1, \ldots, v_m\}$, if $E = \{e_1, \ldots, e_n\}$, then the *incidence matrix* $B(G)$ of G is the $m \times n$ matrix whose entries $b_{i\,j}$ are given by

$$b_{i\,j} = \begin{cases} +1 & \text{if } s(e_j) = v_i \\ -1 & \text{if } t(e_j) = v_i \\ 0 & \text{otherwise.} \end{cases}$$

Here is the incidence matrix of the graph G_1:

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

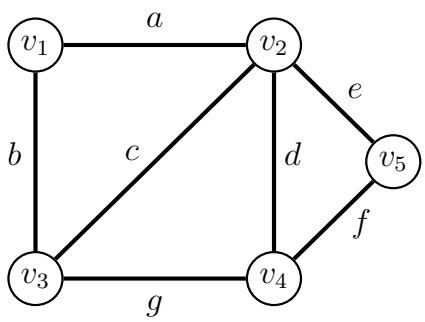

Figure 2.2: The undirected graph G_2.

Observe that every column of an incidence matrix contains exactly two nonzero entries, $+1$ and -1. Again, unless confusion arises, we write B instead of $B(G)$.

When a directed graph has m nodes $v_1, \ldots, v_m$ and n edges $e_1, \ldots, e_n$, a vector $x \in \mathbb{R}^m$ can be viewed as a function $x\colon V \to \mathbb{R}$ assigning the value x_i to the node v_i. Under this interpretation, $\mathbb{R}^m$ is viewed as $\mathbb{R}^V$. Similarly, a vector $y \in \mathbb{R}^n$ can be viewed as a function in $\mathbb{R}^E$. This point of view is often useful. For example, the incidence matrix B can be interpreted as a linear map from $\mathbb{R}^E$ to $\mathbb{R}^V$, the *boundary map*, and $B^\top$ can be interpreted as a linear map from $\mathbb{R}^V$ to $\mathbb{R}^E$, the *coboundary map*.

Remark: Some authors adopt the opposite convention of sign in defining the incidence matrix, which means that their incidence matrix is $-B$.

Undirected graphs are obtained from directed graphs by forgetting the orientation of the edges.

Definition 2.4. A *graph* (or *undirected graph*) is a pair $G = (V, E)$, where $V = \{v_1, \ldots, v_m\}$ is a set of *nodes* or *vertices*, and E is a set of two-element subsets of V (that is, subsets $\{u, v\}$, with $u, v \in V$ and $u \neq v$), called *edges*.

Remark: Since an edge is a set $\{u, v\}$, we have $u \neq v$, so self-loops are not allowed. Also, for every set of nodes $\{u, v\}$, there is at most one edge between u and v. As in the case of directed graphs, such graphs are sometimes called *simple graphs*.

An example of a graph is shown in Figure 2.2.

For every node $v \in V$, the *degree* $d(v)$ of v is the number of edges incident to v:

$$d(v) = |\{u \in V \mid \{u, v\} \in E\}|.$$

The degree matrix D is defined as before.

Definition 2.5. Given a (undirected) graph $G = (V, E)$, for any two nodes $u, v \in V$, a *path from u to v* is a sequence of nodes $(v_0, v_1, \ldots, v_k)$ such that $v_0 = u$, $v_k = v$, and $\{v_i, v_{i+1}\}$ is an edge in E for all i with $0 \leq i \leq k-1$. The integer k is the *length* of the path. A path is *closed* if $u = v$. The graph G is *connected* if for any two distinct nodes $u, v \in V$, there is a path from u to v.

Remark: The terminology *walk* or *chain* is often used instead of *path*, the word path being reserved to the case where the nodes v_i are all distinct, except that $v_0 = v_k$ when the path is closed.

The binary relation on $V \times V$ defined so that u and v are related iff there is a path from u to v is an equivalence relation whose equivalence classes are called the *connected components* of G.

The notion of incidence matrix for an undirected graph is not as useful as in the case of directed graphs

Definition 2.6. Given a graph $G = (V, E)$, with $V = \{v_1, \ldots, v_m\}$, if $E = \{e_1, \ldots, e_n\}$, then the *incidence matrix* $B(G)$ of G is the $m \times n$ matrix whose entries $b_{i\,j}$ are given by

$$b_{i\,j} = \begin{cases} +1 & \text{if } e_j = \{v_i, v_k\} \text{ for some } k \\ 0 & \text{otherwise.} \end{cases}$$

Unlike the case of directed graphs, the entries in the incidence matrix of a graph (undirected) are nonnegative. We usually write B instead of $B(G)$.

The notion of adjacency matrix is basically the same for directed or undirected graphs.

Definition 2.7. Given a directed or undirected graph $G = (V, E)$, with $V = \{v_1, \ldots, v_m\}$, the *adjacency matrix* $A(G)$ of G is the symmetric $m \times m$ matrix $(a_{i\,j})$ such that

(1) If G is directed, then

$$a_{i\,j} = \begin{cases} 1 & \text{if there is some edge } (v_i, v_j) \in E \text{ or some edge } (v_j, v_i) \in E \\ 0 & \text{otherwise.} \end{cases}$$

(2) Else if G is undirected, then

$$a_{i\,j} = \begin{cases} 1 & \text{if there is some edge } \{v_i, v_j\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

As usual, unless confusion arises, we write A instead of $A(G)$. Here is the adjacency matrix of both graphs G_1 and G_2:

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

If $G = (V, E)$ is a directed or an undirected graph, given a node $u \in V$, any node $v \in V$ such that there is an edge (u, v) in the directed case or $\{u, v\}$ in the undirected case is called *adjacent to* u, and we often use the notation

$$u \sim v.$$

Observe that the binary relation $\sim$ is symmetric when G is an undirected graph, but in general it is not symmetric when G is a directed graph.

If $G = (V, E)$ is an undirected graph, the adjacency matrix A of G can be viewed as a linear map from $\mathbb{R}^V$ to $\mathbb{R}^V$, such that for all $x \in \mathbb{R}^m$, we have

$$(Ax)_i = \sum_{j \sim i} x_j;$$

that is, the value of Ax at v_i is the sum of the values of x at the nodes v_j adjacent to v_i. The adjacency matrix can be viewed as a *diffusion operator*. This observation yields a geometric interpretation of what it means for a vector $x \in \mathbb{R}^m$ to be an eigenvector of A associated with some eigenvalue λ; we must have

$$\lambda x_i = \sum_{j \sim i} x_j, \quad i = 1, \ldots, m,$$

which means that the the sum of the values of x assigned to the nodes v_j adjacent to v_i is equal to λ times the value of x at v_i.

Definition 2.8. Given any undirected graph $G = (V, E)$, an *orientation* of G is a function $\sigma \colon E \to V \times V$ assigning a source and a target to every edge in E, which means that for every edge $\{u, v\} \in E$, either $\sigma(\{u, v\}) = (u, v)$ or $\sigma(\{u, v\}) = (v, u)$. The *oriented graph* G^σ obtained from G by applying the orientation σ is the directed graph $G^\sigma = (V, E^\sigma)$, with $E^\sigma = \sigma(E)$.

The following result shows how the number of connected components of an undirected graph is related to the rank of the incidence matrix of any oriented graph obtained from G.

Proposition 2.1. *Let $G = (V, E)$ be any undirected graph with m vertices, n edges, and c connected components. For any orientation σ of G, if B is the incidence matrix of the oriented graph G^σ, then $c = \dim(\mathrm{Ker}\,(B^\top))$, and B has rank $m - c$. Furthermore, the nullspace of $B^\top$ has a basis consisting of indicator vectors of the connected components of G; that is, vectors $(z_1, \ldots, z_m)$ such that $z_j = 1$ iff v_j is in the ith component K_i of G, and $z_j = 0$ otherwise.*

Proof. After Godsil and Royle [10], Section 8.3). The fact that $\text{rank}(B) = m - c$ will be proved last.

Let us prove that the kernel of $B^\top$ has dimension c. A vector $z \in \mathbb{R}^m$ belongs to the kernel of $B^\top$ iff $B^\top z = 0$ iff $z^\top B = 0$. In view of the definition of B, for every edge $\{v_i, v_j\}$ of G, the column of B corresponding to the oriented edge $\sigma(\{v_i, v_j\})$ has zero entries except for a $+1$ and a -1 in position i and position j or vice-versa, so we have

$$z_i = z_j.$$

An easy induction on the length of the path shows that if there is a path from v_i to v_j in G (unoriented), then $z_i = z_j$. Therefore, z has a constant value on any connected component of G. It follows that every vector $z \in \text{Ker}\,(B^\top)$ can be written uniquely as a linear combination

$$z = \lambda_1 z^1 + \cdots + \lambda_c z^c,$$

where the vector z^i corresponds to the ith connected component K_i of G and is defined such that

$$z^i_j = \begin{cases} 1 & \text{iff } v_j \in K_i \\ 0 & \text{otherwise.} \end{cases}$$

This shows that $\dim(\text{Ker}\,(B^\top)) = c$, and that $\text{Ker}\,(B^\top)$ has a basis consisting of indicator vectors.

Since $B^\top$ is a $n \times m$ matrix, we have

$$m = \dim(\text{Ker}\,(B^\top)) + \text{rank}(B^\top),$$

and since we just proved that $\dim(\text{Ker}\,(B^\top)) = c$, we obtain $\text{rank}(B^\top) = m - c$. Since B and $B^\top$ have the same rank, $\text{rank}(B) = m - c$, as claimed. □

Following common practice, we denote by $\mathbf{1}$ the (column) vector whose components are all equal to 1. Since every column of B contains a single $+1$ and a single -1, the rows of $B^\top$ sum to zero, which can be expressed as

$$B^\top \mathbf{1} = 0.$$

According to Proposition 2.1, the graph G is connected iff B has rank $m-1$ iff the nullspace of $B^\top$ is the one-dimensional space spanned by $\mathbf{1}$.

In many applications, the notion of graph needs to be generalized to capture the intuitive idea that two nodes u and v are linked with a degree of certainty (or strength). Thus, we assign a nonnegative weight w_{ij} to an edge $\{v_i, v_j\}$; the smaller w_{ij} is, the weaker is the link (or similarity) between v_i and v_j, and the greater w_{ij} is, the stronger is the link (or similarity) between v_i and v_j.

Definition 2.9. A *weighted graph* is a pair $G = (V, W)$, where $V = \{v_1, \ldots, v_m\}$ is a set of *nodes* or *vertices*, and W is a symmetric matrix called the *weight matrix*, such that $w_{ij} \geq 0$ for all $i, j \in \{1, \ldots, m\}$, and $w_{ii} = 0$ for $i = 1, \ldots, m$. We say that a set $\{v_i, v_j\}$ is an edge iff $w_{ij} > 0$. The corresponding (undirected) graph (V, E) with $E = \{\{v_i, v_j\} \mid w_{ij} > 0\}$, is called the *underlying graph* of G.

Remark: Since $w_{ii} = 0$, these graphs have no self-loops. We can think of the matrix W as a generalized adjacency matrix. The case where $w_{ij} \in \{0, 1\}$ is equivalent to the notion of a graph as in Definition 2.4.

We can think of the weight w_{ij} of an edge $\{v_i, v_j\}$ as a degree of similarity (or affinity) in an image, or a cost in a network. An example of a weighted graph is shown in Figure 2.3. The thickness of an edge corresponds to the magnitude of its weight.

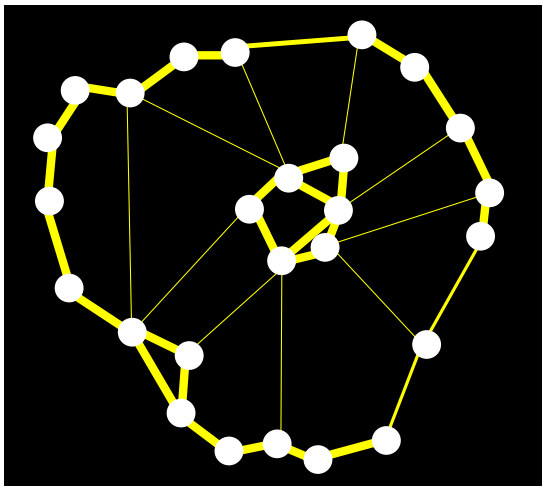

Figure 2.3: A weighted graph.

For every node $v_i \in V$, the *degree* $d(v_i)$ of v_i is the sum of the weights of the edges adjacent to v_i:

$$d(v_i) = \sum_{j=1}^{m} w_{ij}.$$

Note that in the above sum, only nodes v_j such that there is an edge $\{v_i, v_j\}$ have a nonzero contribution. Such nodes are said to be *adjacent* to v_i, and we write $v_i \sim v_j$. The degree matrix D is defined as before, namely by $D = \mathrm{diag}(d(v_1), \ldots, d(v_m))$.

The weight matrix W can be viewed as a linear map from $\mathbb{R}^V$ to itself. For all $x \in \mathbb{R}^m$, we have

$$(Wx)_i = \sum_{j \sim i} w_{ij} x_j;$$

that is, the value of Wx at v_i is the weighted sum of the values of x at the nodes v_j adjacent to v_i.

Observe that $W\mathbf{1}$ is the (column) vector $(d(v_1), \ldots, d(v_m))$ consisting of the degrees of the nodes of the graph.

Given any subset of nodes $A \subseteq V$, we define the *volume* $\mathrm{vol}(A)$ of A as the sum of the weights of all edges adjacent to nodes in A:

$$\mathrm{vol}(A) = \sum_{v_i \in A} d(v_i) = \sum_{v_i \in A} \sum_{j=1}^{m} w_{ij}.$$

Remark: Yu and Shi [24] use the notation $\mathrm{degree}(A)$ instead of $\mathrm{vol}(A)$.

The notions of degree and volume are illustrated in Figure 2.4.

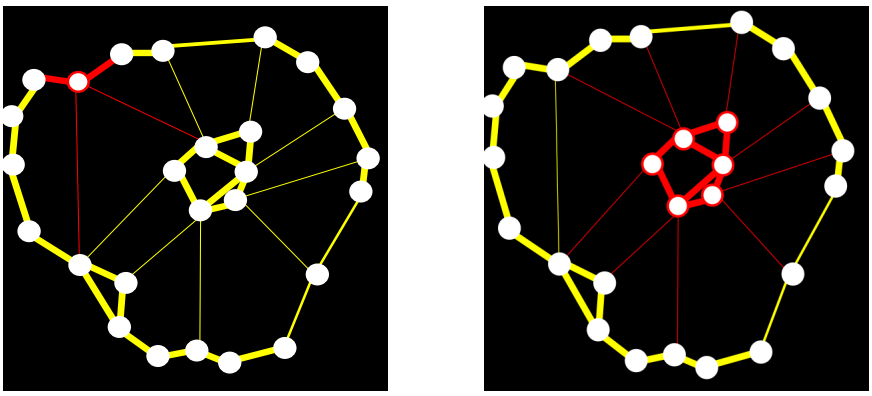

Figure 2.4: Degree and volume.

Observe that $\mathrm{vol}(A) = 0$ if A consists of isolated vertices, that is, if $w_{ij} = 0$ for all $v_i \in A$. Thus, it is best to assume that G does not have isolated vertices.

Given any two subset $A, B \subseteq V$ (not necessarily distinct), we define $\mathrm{links}(A, B)$ by

$$\mathrm{links}(A, B) = \sum_{v_i \in A, v_j \in B} w_{ij}.$$

Since the matrix W is symmetric, we have

$$\mathrm{links}(A, B) = \mathrm{links}(B, A),$$

and observe that $\mathrm{vol}(A) = \mathrm{links}(A, V)$.

The quantity $\mathrm{links}(A, \overline{A}) = \mathrm{links}(\overline{A}, A)$ (where $\overline{A} = V - A$ denotes the complement of A in V) measures how many links escape from A (and $\overline{A}$), and the quantity $\mathrm{links}(A, A)$ measures how many links stay within A itself. The quantity

$$\mathrm{cut}(A) = \mathrm{links}(A, \overline{A})$$

is often called the *cut* of A, and the quantity

$$\text{assoc}(A) = \text{links}(A, A)$$

is often called the *association* of A. Clearly,

$$\text{cut}(A) + \text{assoc}(A) = \text{vol}(A).$$

The notion of cut is illustrated in Figure 2.5.

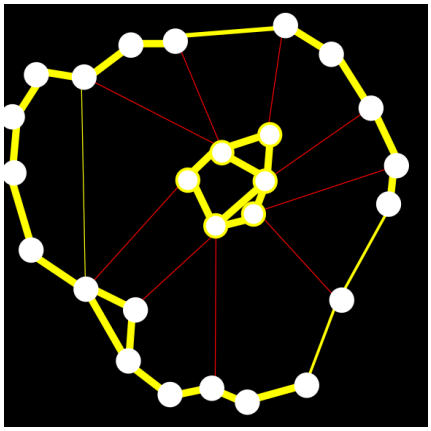

Figure 2.5: A Cut involving the set of nodes in the center and the nodes on the perimeter.

We now define the most important concept of these notes: The Laplacian matrix of a graph. Actually, as we will see, it comes in several flavors.

2.2 Laplacian Matrices of Graphs

Let us begin with directed graphs, although as we will see, graph Laplacians are fundamentally associated with undirected graph. The key proposition below shows how given an undirected graph G, for any orientation σ of G, $B^\sigma(B^\sigma)^\top$ relates to the adjacency matrix A (where B^σ is the incidence matrix of the directed graph G^σ). We reproduce the proof in Gallier [7] (see also Godsil and Royle [10]).

Proposition 2.2. *Given any undirected graph G, for any orientation σ of G, if B^σ is the incidence matrix of the directed graph G^σ, A is the adjacency matrix of G^σ, and D is the degree matrix such that $D_{ii} = d(v_i)$, then*

$$B^\sigma(B^\sigma)^\top = D - A.$$

Consequently, $L = B^\sigma(B^\sigma)^\top$ is independent of the orientation σ of G, and $D-A$ is symmetric and positive semidefinite; that is, the eigenvalues of $D - A$ are real and nonnegative.

Proof. The entry $B^\sigma(B^\sigma)^\top_{ij}$ is the inner product of the ith row b_i^σ, and the jth row b_j^σ of B^σ. If $i = j$, then as

$$b^\sigma_{i\,k} = \begin{cases} +1 & \text{if } s(e_k) = v_i \\ -1 & \text{if } t(e_k) = v_i \\ 0 & \text{otherwise} \end{cases}$$

we see that $b_i^\sigma \cdot b_i^\sigma = d(v_i)$. If $i \neq j$, then $b_i^\sigma \cdot b_j^\sigma \neq 0$ iff there is some edge e_k with $s(e_k) = v_i$ and $t(e_k) = v_j$ or vice-versa (which are mutually exclusive cases, since G^σ arises by orienting an undirected graph), in which case, $b_i^\sigma \cdot b_j^\sigma = -1$. Therefore,

$$B^\sigma(B^\sigma)^\top = D - A,$$

as claimed.

For every $x \in \mathbb{R}^m$, we have

$$x^\top L x = x^\top B^\sigma (B^\sigma)^\top x = ((B^\sigma)^\top x)^\top (B^\sigma)^\top x = \left\|(B^\sigma)^\top x\right\|_2^2 \geq 0,$$

since the Euclidean norm $\| \ \|_2$ is positive (definite). Therefore, $L = B^\sigma(B^\sigma)^\top$ is positive semidefinite. It is well-known that a real symmetric matrix is positive semidefinite iff its eigenvalues are nonnegtive. □

The matrix $L = B^\sigma(B^\sigma)^\top = D - A$ is called the *(unnormalized) graph Laplacian* of the graph G^σ. For example, the graph Laplacian of graph G_1 is

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

The *(unnormalized) graph Laplacian* of an undirected graph $G = (V, E)$ is defined by

$$L = D - A.$$

Observe that each row of L sums to zero (because $(B^\sigma)^\top \mathbf{1} = 0$). Consequently, the vector $\mathbf{1}$ is in the nullspace of L.

Remarks:

1. With the unoriented version of the incidence matrix (see Definition 2.6), it can be shown that
$$BB^\top = D + A.$$

2. As pointed out by Evangelos Chatzipantazis, Proposition 2.2 in which the incidence matrix B^σ is replaced by the incidence matrix B of any *arbitrary* directed graph G does not hold. The problem is that such graphs may have both edges (v_i, v_j) and (v_j, v_i) between two distinct nodes v_i and v_j, and as a consequence, the inner product $b_i \cdot b_j = -2$ instead of -1. A simple counterexample is given by the directed graph with three vertices and four edges whose incidence matrix is given by

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

We have

$$BB^\top = \begin{pmatrix} 3 & -2 & -1 \\ -2 & 3 & -1 \\ -1 & -1 & 2 \end{pmatrix} \neq \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} = D - A.$$

The natural generalization of the notion of graph Laplacian to weighted graphs is this:

Definition 2.10. Given any weighted graph $G = (V, W)$ with $V = \{v_1, \ldots, v_m\}$, the *(unnormalized) graph Laplacian $L(G)$ of G* is defined by

$$L(G) = D(G) - W,$$

where $D(G) = \mathrm{diag}(d_1, \ldots, d_m)$ is the degree matrix of G (a diagonal matrix), with

$$d_i = \sum_{j=1}^{m} w_{i\,j}.$$

As usual, unless confusion arises, we write L instead of $L(G)$.

The graph Laplacian can be interpreted as a linear map from $\mathbb{R}^V$ to itself. For all $x \in \mathbb{R}^V$, we have

$$(Lx)_i = \sum_{j \sim i} w_{ij}(x_i - x_j).$$

It is clear that each row of L sums to 0, so the vector $\mathbf{1}$ is the nullspace of L, but it is less obvious that L is positive semidefinite. One way to prove it is to generalize slightly the notion of incidence matrix.

Definition 2.11. Given a weighted graph $G = (V, W)$, with $V = \{v_1, \ldots, v_m\}$, if $\{e_1, \ldots, e_n\}$ are the edges of the underlying graph of G (recall that $\{v_i, v_j\}$ is an edge of this graph iff $w_{ij} > 0$), for any oriented graph G^σ obtained by giving an orientation to the underlying graph of G, the *incidence matrix* B^σ of G^σ is the $m \times n$ matrix whose entries $b_{i\,j}$ are given by

$$b_{i\,j} = \begin{cases} +\sqrt{w_{ij}} & \text{if } s(e_j) = v_i \\ -\sqrt{w_{ij}} & \text{if } t(e_j) = v_i \\ 0 & \text{otherwise.} \end{cases}$$

For example, given the weight matrix

$$W = \begin{pmatrix} 0 & 3 & 6 & 3 \\ 3 & 0 & 0 & 3 \\ 6 & 0 & 0 & 3 \\ 3 & 3 & 3 & 0 \end{pmatrix},$$

the incidence matrix B corresponding to the orientation of the underlying graph of W where an edge (i, j) is oriented positively iff $i < j$ is

$$B = \begin{pmatrix} 1.7321 & 2.4495 & 1.7321 & 0 & 0 \\ -1.7321 & 0 & 0 & 1.7321 & 0 \\ 0 & -2.4495 & 0 & 0 & 1.7321 \\ 0 & 0 & -1.7321 & -1.7321 & -1.7321 \end{pmatrix}.$$

The reader should verify that $BB^\top = D - W$. This is true in general, see Proposition 2.3.

It is easy to see that Proposition 2.1 applies to the underlying graph of G. For any oriented graph G^σ obtained from the underlying graph of G, the rank of the incidence matrix B^σ is equal to $m - c$, where c is the number of connected components of the underlying graph of G, and we have $(B^\sigma)^\top \mathbf{1} = 0$. We also have the following version of Proposition 2.2 whose proof is immediately adapted.

Proposition 2.3. *Given any weighted graph $G = (V, W)$ with $V = \{v_1, \ldots, v_m\}$, if B^σ is the incidence matrix of any oriented graph G^σ obtained from the underlying graph of G and D is the degree matrix of W, then*

$$B^\sigma (B^\sigma)^\top = D - W = L.$$

Consequently, $B^\sigma (B^\sigma)^\top$ is independent of the orientation of the underlying graph of G and $L = D - W$ is symmetric and positive semidefinite; that is, the eigenvalues of $L = D - W$ are real and nonnegative.

Remark: Given any orientation G^σ of the underlying graph of a weighted graph $G = (V, W)$, if B is the incidence matrix of G^σ, then $B^\top$ defines a kind of discrete covariant derivative $\nabla \colon \mathbb{R}^V \times \mathcal{X}(G) \to \mathbb{R}^V$ on the set of 0-forms, which is just the set of functions $\mathbb{R}^V$. For every vertex $v_i \in V$, we view the set of edges with source or endpoint v_i,

$$T_{v_i} G = \{(v_i, v_j) \mid w_{ij} \neq 0\} \cup \{(v_h, v_i) \mid w_{hi} \neq 0\},$$

as a kind of discrete tangent space at v_i. The disjoint union of the tangent spaces $T_{v_i} G$ is the discrete tangent bundle TG. A discrete vector field is then a function $X \colon V \to TG$ that assigns to every vertex $v_i \in V$ some edge $X(v_i) = e_k \in T_{v_i} G$, and we denote the set of all discrete vectors fields by $\mathcal{X}(G)$. For every function $f \in \mathbb{R}^V$ and for every vector field

$X \in \mathcal{X}(G)$, we define the function $\nabla_X f$, a discrete analog of the covariant derivative of the function f with respect to the vector field X, by

$$(\nabla_X f)(v_i) = B^\top(f)(X(v_i));$$

that is, if $X(v_i)$ is the kth edge $e_k = (v_i, v_j)$, then

$$(\nabla_X f)(v_i) = \sqrt{w_{ij}}(f_i - f_j),$$

else if $X(v_i)$ is the kth edge $e_k = (v_j, v_i)$, then

$$(\nabla_X f)(v_i) = \sqrt{w_{ij}}(f_j - f_i).$$

Then, the graph Laplacian L is given by

$$L = BB^\top;$$

for every node v_i, we have

$$(Lx)_i = \sum_{j \sim i} w_{ij}(x_i - x_j).$$

Thus, L appears to be a discrete analog of the *connection Laplacian* (also known as *Bochner Laplacian*), rather than a discrete analog of the Hodge (Laplace–Beltrami) Laplacian; see Petersen [19]. To make the above statement precise, we need to view ∇f as the function from $\mathcal{X}(G)$ to $\mathbb{R}^V$ given by

$$(\nabla f)(X) = \nabla_X f.$$

The set of functions from $\mathcal{X}(G)$ to $\mathbb{R}^V$ is in bijection with the set of functions $\mathbb{R}^{\mathcal{X}(G)\times V}$ from $\mathcal{X}(G) \times V$ to $\mathbb{R}$, and we can view the discrete connection ∇ as a linear map $\nabla\colon \mathbb{R}^V \to \mathbb{R}^{\mathcal{X}(G)\times V}$. Since both $\mathcal{X}(G)$ and V are finite, we can use the inner product on the vector space $\mathbb{R}^{\mathcal{X}(G)\times V}$ (and the inner product on $\mathbb{R}^V$) to define the adjoint $\nabla^*\colon \mathbb{R}^{\mathcal{X}(G)\times V} \to \mathbb{R}^V$ of $\nabla\colon \mathbb{R}^V \to \mathbb{R}^{\mathcal{X}(G)\times V}$ by

$$\langle \nabla^* F, f\rangle = \langle F, \nabla f\rangle,$$

for all $f \in \mathbb{R}^V$ and all $F \in \mathbb{R}^{\mathcal{X}(G)\times V}$. Then, the connection Laplacian $\nabla^*\nabla\colon \mathbb{R}^V \to \mathbb{R}^V$ is indeed equal to L.

Another way to prove that L is positive semidefinite is to evaluate the quadratic form $x^\top Lx$.

Proposition 2.4. *For any $m \times m$ symmetric matrix $W = (w_{ij})$, if we let $L = D - W$ where D is the degree matrix associated with W, then we have*

$$x^\top Lx = \frac{1}{2}\sum_{i,j=1}^{m} w_{ij}(x_i - x_j)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

Consequently, $x^\top Lx$ does not depend on the diagonal entries in W, and if $w_{ij} \geq 0$ for all $i, j \in \{1, \ldots, m\}$, then L is positive semidefinite.

Proof. We have

$$\begin{aligned} x^\top Lx &= x^\top Dx - x^\top Wx \\ &= \sum_{i=1}^m d_i x_i^2 - \sum_{i,j=1}^m w_{ij} x_i x_j \\ &= \frac{1}{2}\left(\sum_{i=1}^m d_i x_i^2 - 2\sum_{i,j=1}^m w_{ij} x_i x_j + \sum_{i=1}^m d_i x_i^2\right) \\ &= \frac{1}{2}\sum_{i,j=1}^m w_{ij}(x_i - x_j)^2. \end{aligned}$$

Obviously, the quantity on the right-hand side does not depend on the diagonal entries in W, and if $w_{ij} \geq 0$ for all i, j, then this quantity is nonnegative. □

Proposition 2.4 immediately implies the following facts: For any weighted graph $G = (V, W)$,

1. The eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_m$ of L are real and nonnegative, and there is an orthonormal basis of eigenvectors of L.

2. The smallest eigenvalue λ_1 of L is equal to 0, and $\mathbf{1}$ is a corresponding eigenvector.

It turns out that the dimension of the nullspace of L (the eigenspace of 0) is equal to the number of connected components of the underlying graph of G.

Proposition 2.5. *Let $G = (V, W)$ be a weighted graph. The number c of connected components $K_1, \ldots, K_c$ of the underlying graph of G is equal to the dimension of the nullspace of L, which is equal to the multiplicity of the eigenvalue 0. Furthermore, the nullspace of L has a basis consisting of indicator vectors of the connected components of G, that is, vectors $(f_1, \ldots, f_m)$ such that $f_j = 1$ iff $v_j \in K_i$ and $f_j = 0$ otherwise.*

Proof. Since $L = BB^\top$ for the incidence matrix B associated with any oriented graph obtained from G, and since L and $B^\top$ have the same nullspace, by Proposition 2.1, the dimension of the nullspace of L is equal to the number c of connected components of G and the indicator vectors of the connected components of G form a basis of $\mathrm{Ker}\,(L)$. □

Proposition 2.5 implies that if the underlying graph of G is connected, then the second eigenvalue λ_2 of L is strictly positive.

Remarkably, the eigenvalue λ_2 contains a lot of information about the graph G (assuming that $G = (V, E)$ is an undirected graph). This was first discovered by Fiedler in 1973, and for this reason, λ_2 is often referred to as the *Fiedler number*. For more on the properties of the Fiedler number, see Godsil and Royle [10] (Chapter 13) and Chung [4]. More generally, the

spectrum $(0, \lambda_2, \ldots, \lambda_m)$ of L contains a lot of information about the combinatorial structure of the graph G. Leverage of this information is the object of *spectral graph theory*.

It turns out that normalized variants of the graph Laplacian are needed, especially in applications to graph clustering. These variants make sense only if G has no isolated vertices, which means that every row of W contains some strictly positive entry. In this case, the degree matrix D contains positive entries, so it is invertible and $D^{-1/2}$ makes sense; namely

$$D^{-1/2} = \mathrm{diag}(d_1^{-1/2}, \ldots, d_m^{-1/2}),$$

and similarly for any real exponent α.

Definition 2.12. Given any weighted directed graph $G = (V, W)$ with no isolated vertex and with $V = \{v_1, \ldots, v_m\}$, the *(normalized) graph Laplacians* L_{sym} *and* L_{rw} *of* G are defined by

$$\begin{aligned} L_{\mathrm{sym}} &= D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2} \\ L_{\mathrm{rw}} &= D^{-1} L = I - D^{-1} W. \end{aligned}$$

Observe that the Laplacian $L_{\mathrm{sym}} = D^{-1/2} L D^{-1/2}$ is a symmetric matrix (because L and $D^{-1/2}$ are symmetric) and that

$$L_{\mathrm{rw}} = D^{-1/2} L_{\mathrm{sym}} D^{1/2}.$$

The reason for the notation L_{rw} is that this matrix is closely related to a random walk on the graph G.

Since the unnormalized Laplacian L can be written as $L = BB^\top$, where B is the incidence matrix of any oriented graph obtained from the underlying graph of $G = (V, W)$, if we let

$$B_{\mathrm{sym}} = D^{-1/2} B,$$

we get

$$L_{\mathrm{sym}} = B_{\mathrm{sym}} B_{\mathrm{sym}}^\top.$$

In particular, for any singular decomposition $B_{\mathrm{sym}} = U \Sigma V^\top$ of B_{sym} (with U an $m \times m$ orthogonal matrix, Σ a "diagonal" $m \times n$ matrix of singular values, and V an $n \times n$ orthogonal matrix), the eigenvalues of L_{sym} are the squares of the top m singular values of B_{sym}, and the vectors in U are orthonormal eigenvectors of L_{sym} with respect to these eigenvalues (the squares of the top m diagonal entries of Σ). Computing the SVD of B_{sym} generally yields more accurate results than diagonalizing L_{sym}, especially when L_{sym} has eigenvalues with high multiplicity.

There are simple relationships between the eigenvalues and the eigenvectors of L_{sym}, and L_{rw}. There is also a simple relationship with the generalized eigenvalue problem $Lx = \lambda D x$.

Proposition 2.6. *Let $G = (V, W)$ be a weighted graph without isolated vertices. The graph Laplacians, L, L_{sym}, and L_{rw} satisfy the following properties:*

(1) The matrix L_{sym} is symmetric and positive semidefinite. In fact,

$$x^\top L_{\mathrm{sym}} x = \frac{1}{2}\sum_{i,j=1}^{m} w_{ij}\left(\frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}}\right)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

(2) The normalized graph Laplacians L_{sym} and L_{rw} have the same spectrum $(0 = \nu_1 \leq \nu_2 \leq \ldots \leq \nu_m)$, and a vector $u \neq 0$ is an eigenvector of L_{rw} for λ iff $D^{1/2}u$ is an eigenvector of L_{sym} for λ.

(3) The graph Laplacians L and L_{sym} are symmetric and positive semidefinite.

(4) A vector $u \neq 0$ is a solution of the generalized eigenvalue problem $Lu = \lambda Du$ iff $D^{1/2}u$ is an eigenvector of L_{sym} for the eigenvalue λ iff u is an eigenvector of L_{rw} for the eigenvalue λ.

(5) The graph Laplacians, L and L_{rw} have the same nullspace. For any vector u, we have $u \in \mathrm{Ker}\,(L)$ iff $D^{1/2}u \in \mathrm{Ker}\,(L_{\mathrm{sym}})$.

(6) The vector $\mathbf{1}$ is in the nullspace of L_{rw}, and $D^{1/2}\mathbf{1}$ is in the nullspace of L_{sym}.

(7) For every eigenvalue ν_i of the normalized graph Laplacian L_{sym}, we have $0 \leq \nu_i \leq 2$. Furthermore, $\nu_m = 2$ iff the underlying graph of G contains a nontrivial connected bipartite component.

(8) If $m \geq 2$ and if the underlying graph of G is not a complete graph, then $\nu_2 \leq 1$. Furthermore the underlying graph of G is a complete graph iff $\nu_2 = \frac{m}{m-1}$.

(9) If $m \geq 2$ and if the underlying graph of G is connected then $\nu_2 > 0$.

(10) If $m \geq 2$ and if the underlying graph of G has no isolated vertices, then $\nu_m \geq \frac{m}{m-1}$.

Proof. (1) We have $L_{\mathrm{sym}} = D^{-1/2}LD^{-1/2}$, and $D^{-1/2}$ is a symmetric invertible matrix (since it is an invertible diagonal matrix). It is a well-known fact of linear algebra that if B is an invertible matrix, then a matrix S is symmetric, positive semidefinite iff $BSB^\top$ is symmetric, positive semidefinite. Since L is symmetric, positive semidefinite, so is $L_{\mathrm{sym}} = D^{-1/2}LD^{-1/2}$. The formula

$$x^\top L_{\mathrm{sym}} x = \frac{1}{2}\sum_{i,j=1}^{m} w_{ij}\left(\frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}}\right)^2 \quad \text{for all } x \in \mathbb{R}^m$$

follows immediately from Proposition 2.4 by replacing x by $D^{-1/2}x$, and also shows that L_{sym} is positive semidefinite.

(2) Since

$$L_{\mathrm{rw}} = D^{-1/2} L_{\mathrm{sym}} D^{1/2},$$

the matrices L_{sym} and L_{rw} are similar, which implies that they have the same spectrum. In fact, since $D^{1/2}$ is invertible,

$$L_{\mathrm{rw}} u = D^{-1} L u = \lambda u$$

iff

$$D^{-1/2} L u = \lambda D^{1/2} u$$

iff

$$D^{-1/2} L D^{-1/2} D^{1/2} u = L_{\mathrm{sym}} D^{1/2} u = \lambda D^{1/2} u,$$

which shows that a vector $u \neq 0$ is an eigenvector of L_{rw} for λ iff $D^{1/2}u$ is an eigenvector of L_{sym} for λ.

(3) We already know that L and L_{sym} are positive semidefinite.

(4) Since $D^{-1/2}$ is invertible, we have

$$L u = \lambda D u$$

iff

$$D^{-1/2} L u = \lambda D^{1/2} u$$

iff

$$D^{-1/2} L D^{-1/2} D^{1/2} u = L_{\mathrm{sym}} D^{1/2} u = \lambda D^{1/2} u,$$

which shows that a vector $u \neq 0$ is a solution of the generalized eigenvalue problem $Lu = \lambda Du$ iff $D^{1/2}u$ is an eigenvector of L_{sym} for the eigenvalue λ. The second part of the statement follows from (2).

(5) Since D^{-1} is invertible, we have $Lu = 0$ iff $D^{-1}Lu = L_{\mathrm{rw}}u = 0$. Similarly, since $D^{-1/2}$ is invertible, we have $Lu = 0$ iff $D^{-1/2}LD^{-1/2}D^{1/2}u = 0$ iff $D^{1/2}u \in \mathrm{Ker}\,(L_{\mathrm{sym}})$.

(6) Since $L\mathbf{1} = 0$, we get $L_{\mathrm{rw}}\mathbf{1} = D^{-1}L\mathbf{1} = 0$. That $D^{1/2}\mathbf{1}$ is in the nullspace of L_{sym} follows from (2). Properties (7)–(10) are proved in Chung [4] (Chapter 1). □

Remark: Observe that although the matrices L_{sym} and L_{rw} have the same spectrum, the matrix L_{rw} is generally not symmetric, whereas L_{sym} is symmetric.

A version of Proposition 2.5 also holds for the graph Laplacians L_{sym} and L_{rw}. This follows easily from the fact that Proposition 2.1 applies to the underlying graph of a weighted graph. The proof is left as an exercise.

Proposition 2.7. *Let $G = (V, W)$ be a weighted graph. The number c of connected components $K_1, \ldots, K_c$ of the underlying graph of G is equal to the dimension of the nullspace of both L_{sym} and L_{rw}, which is equal to the multiplicity of the eigenvalue 0. Furthermore, the nullspace of L_{rw} has a basis consisting of indicator vectors of the connected components of G, that is, vectors $(f_1, \ldots, f_m)$ such that $f_j = 1$ iff $v_j \in K_i$ and $f_j = 0$ otherwise. For L_{sym}, a basis of the nullpace is obtained by multiplying the above basis of the nullspace of L_{rw} by $D^{1/2}$.*

Chapter 3

Spectral Graph Drawing

3.1 Graph Drawing and Energy Minimization

Let $G = (V, E)$ be some undirected graph. It is often desirable to draw a graph, usually in the plane but possibly in 3D, and it turns out that the graph Laplacian can be used to design surprisingly good methods. Say $|V| = m$. The idea is to assign a point $\rho(v_i)$ in $\mathbb{R}^n$ to the vertex $v_i \in V$, for every $v_i \in V$, and to draw a line segment between the points $\rho(v_i)$ and $\rho(v_j)$ iff there is an edge $\{v_i, v_j\}$. Thus, a *graph drawing* is a function $\rho\colon V \to \mathbb{R}^n$.

We define the *matrix of a graph drawing ρ (in $\mathbb{R}^n$)* as a $m \times n$ matrix R whose ith row consists of the row vector $\rho(v_i)$ corresponding to the point representing v_i in $\mathbb{R}^n$. Typically, we want $n < m$; in fact n should be much smaller than m. A representation is *balanced* iff the sum of the entries of every column is zero, that is,

$$\mathbf{1}^\top R = 0.$$

If a representation is not balanced, it can be made balanced by a suitable translation. We may also assume that the columns of R are linearly independent, since any basis of the column space also determines the drawing. Thus, from now on, we may assume that $n \leq m$.

Remark: A graph drawing $\rho\colon V \to \mathbb{R}^n$ is not required to be injective, which may result in degenerate drawings where distinct vertices are drawn as the same point. For this reason, we prefer not to use the terminology *graph embedding*, which is often used in the literature. This is because in differential geometry, an embedding always refers to an injective map. The term *graph immersion* would be more appropriate.

As explained in Godsil and Royle [10], we can imagine building a physical model of G by connecting adjacent vertices (in $\mathbb{R}^n$) by identical springs. Then, it is natural to consider a representation to be better if it requires the springs to be less extended. We can formalize this by defining the *energy* of a drawing R by

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} \|\rho(v_i) - \rho(v_j)\|^2,$$

where $\rho(v_i)$ is the ith row of R and $\|\rho(v_i) - \rho(v_j)\|^2$ is the square of the Euclidean length of the line segment joining $\rho(v_i)$ and $\rho(v_j)$.

Then, "good drawings" are drawings that minimize the energy function $\mathcal{E}$. Of course, the trivial representation corresponding to the zero matrix is optimum, so we need to impose extra constraints to rule out the trivial solution.

We can consider the more general situation where the springs are not necessarily identical. This can be modeled by a symmetric weight (or stiffness) matrix $W = (w_{ij})$, with $w_{ij} \geq 0$. Then our energy function becomes

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} w_{ij} \|\rho(v_i) - \rho(v_j)\|^2 .$$

It turns out that this function can be expressed in terms of the Laplacian $L = D - W$. The following proposition is shown in Godsil and Royle [10]. We give a slightly more direct proof.

Proposition 3.1. *Let $G = (V, W)$ be a weighted graph, with $|V| = m$ and W an $m \times m$ symmetric matrix, and let R be the matrix of a graph drawing ρ of G in $\mathbb{R}^n$ (a $m \times n$ matrix). If $L = D - W$ is the unnormalized Laplacian matrix associated with W, then*

$$\mathcal{E}(R) = \mathrm{tr}(R^\top L R).$$

Proof. Since $\rho(v_i)$ is the ith row of R (and $\rho(v_j)$ is the jth row of R), if we denote the kth column of R by R^k, using Proposition 2.4, we have

$$\begin{aligned}
\mathcal{E}(R) &= \sum_{\{v_i, v_j\} \in E} w_{ij} \|\rho(v_i) - \rho(v_j)\|^2 \\
&= \sum_{k=1}^{n} \sum_{\{v_i, v_j\} \in E} w_{ij} (R_{ik} - R_{jk})^2 \\
&= \sum_{k=1}^{n} \frac{1}{2} \sum_{i,j=1}^{m} w_{ij} (R_{ik} - R_{jk})^2 \\
&= \sum_{k=1}^{n} (R^k)^\top L R^k = \mathrm{tr}(R^\top L R),
\end{aligned}$$

as claimed. □

Note that

$$L\mathbf{1} = 0,$$

as we already observed.

Since the matrix $R^\top L R$ is symmetric, it has real eigenvalues. Actually, since L is positive semidefinite, so is $R^\top L R$. Then, the trace of $R^\top L R$ is equal to the sum of its positive eigenvalues, and this is the energy $\mathcal{E}(R)$ of the graph drawing.

If R is the matrix of a graph drawing in $\mathbb{R}^n$, then for any invertible matrix M, the map that assigns $\rho(v_i)M$ to v_i is another graph drawing of G, and these two drawings convey the same amount of information. From this point of view, a graph drawing is determined by the column space of R. Therefore, it is reasonable to assume that the columns of R are pairwise orthogonal and that they have unit length. Such a matrix satisfies the equation $R^\top R = I$, and the corresponding drawing is called an *orthogonal drawing*. This condition also rules out trivial drawings. The following result tells us how to find minimum energy orthogonal balanced graph drawings, provided the graph is connected.

Theorem 3.2. *Let $G = (V, W)$ be a weighted graph with $|V| = m$. If $L = D - W$ is the (unnormalized) Laplacian of G, and if the eigenvalues of L are $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_m$, then the minimal energy of any balanced orthogonal graph drawing of G in $\mathbb{R}^n$ is equal to $\lambda_2 + \cdots + \lambda_{n+1}$ (in particular, this implies that $n < m$). The $m \times n$ matrix R consisting of any unit eigenvectors $u_2, \ldots, u_{n+1}$ associated with $\lambda_2 \leq \ldots \leq \lambda_{n+1}$ yields a balanced orthogonal graph drawing of minimal energy; it satisfies the condition $R^\top R = I$.*

Proof. We present the proof given in Godsil and Royle [10] (Section 13.4, Theorem 13.4.1). The key point is that the sum of the n smallest eigenvalues of L is a lower bound for $\mathrm{tr}(R^\top LR)$. This can be shown using an argument using the Rayleigh ratio; see Proposition A.3 (the Poincaré separation theorem). Then, any n eigenvectors $(u_1, \ldots, u_n)$ associated with $\lambda_1, \ldots, \lambda_n$ achieve this bound. Because the first eigenvalue of L is $\lambda_1 = 0$ and because we are assuming that $\lambda_2 > 0$, we have $u_1 = \mathbf{1}/\sqrt{m}$. Since the u_j are pairwise orthogonal for $i = 2, \ldots, n$ and since u_i is orthogonal to $u_1 = \mathbf{1}/\sqrt{m}$, the entries in u_i add up to 0. Consequently, for any ℓ with $2 \leq \ell \leq n$, by deleting u_1 and using $(u_2, \ldots, u_\ell)$, we obtain a balanced orthogonal graph drawing in $\mathbb{R}^{\ell-1}$ with the same energy as the orthogonal graph drawing in $\mathbb{R}^\ell$ using $(u_1, u_2, \ldots, u_\ell)$. Conversely, from any balanced orthogonal drawing in $\mathbb{R}^{\ell-1}$ using $(u_2, \ldots, u_\ell)$, we obtain an orthogonal graph drawing in $\mathbb{R}^\ell$ using $(u_1, u_2, \ldots, u_\ell)$ with the same energy. Therefore, the minimum energy of a balanced orthogonal graph drawing in $\mathbb{R}^n$ is equal to the minimum energy of an orthogonal graph drawing in $\mathbb{R}^{n+1}$, and this minimum is $\lambda_2 + \cdots + \lambda_{n+1}$. □

Since $\mathbf{1}$ spans the nullspace of L, using u_1 (which belongs to $\mathrm{Ker}\, L$) as one of the vectors in R would have the effect that all points representing vertices of G would have the same first coordinate. This would mean that the drawing lives in a hyperplane in $\mathbb{R}^n$, which is undesirable, especially when $n = 2$, where all vertices would be collinear. This is why we omit the first eigenvector u_1.

Observe that for any orthogonal $n \times n$ matrix Q, since

$$\mathrm{tr}(R^\top LR) = \mathrm{tr}(Q^\top R^\top LRQ),$$

the matrix RQ also yields a minimum orthogonal graph drawing. This amounts to applying the rigid motion $Q^\top$ to the rows of R.

In summary, if $\lambda_2 > 0$, an automatic method for drawing a graph in $\mathbb{R}^2$ is this:

1. Compute the two smallest nonzero eigenvalues $\lambda_2 \leq \lambda_3$ of the graph Laplacian L (it is possible that $\lambda_3 = \lambda_2$ if λ_2 is a multiple eigenvalue);

2. Compute two unit eigenvectors u_2, u_3 associated with λ_2 and λ_3, and let $R = [u_2\, u_3]$ be the $m \times 2$ matrix having u_2 and u_3 as columns.

3. Place vertex v_i at the point whose coordinates is the ith row of R, that is, (R_{i1}, R_{i2}).

This method generally gives pleasing results, but beware that there is no guarantee that distinct nodes are assigned distinct images, because R can have identical rows. This does not seem to happen often in practice.

3.2 Examples of Graph Drawings

We now give a number of examples using `Matlab`. Some of these are borrowed or adapted from Spielman [21].

Example 1. Consider the graph with four nodes whose adjacency matrix is

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

We use the following program to compute u_2 and u_3:

```
A = [0 1 1 0; 1 0 0 1; 1 0 0 1; 0 1 1 0];
D = diag(sum(A));
L = D - A;
[v, e] = eigs(L);
gplot(A, v(:,[3 2]))
hold on;
gplot(A, v(:,[3 2]),'o')
```

The graph of Example 1 is shown in Figure 3.1. The function `eigs(L)` computes the six largest eigenvalues of L in decreasing order, and corresponding eigenvectors. It turns out that $\lambda_2 = \lambda_3 = 2$ is a double eigenvalue.

Example 2. Consider the graph G_2 shown in Figure 2.2 given by the adjacency matrix

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

We use the following program to compute u_2 and u_3:

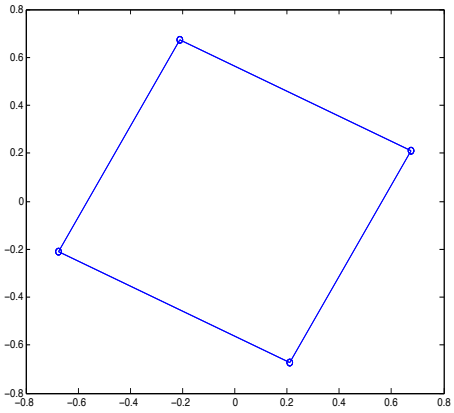

Figure 3.1: Drawing of the graph from Example 1.

```
A = [0 1 1 0 0; 1 0 1 1 1; 1 1 0 1 0; 0 1 1 0 1; 0 1 0 1 0];
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on
gplot(A, v(:, [2 3]),'o')
```

The function `eig(L)` (with no `s` at the end) computes the eigenvalues of L in increasing order. The result of drawing the graph is shown in Figure 3.2. Note that node v_2 is assigned to the point $(0, 0)$, so the difference between this drawing and the drawing in Figure 2.2 is that the drawing of Figure 3.2 is not convex.

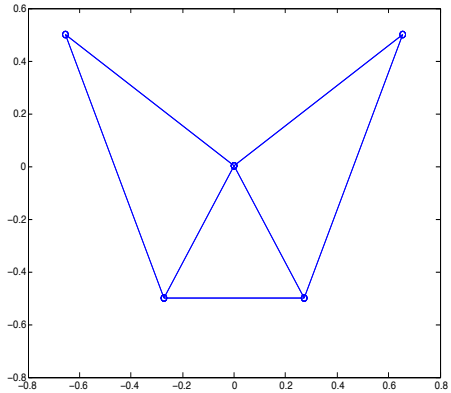

Figure 3.2: Drawing of the graph from Example 2.

Example 3. Consider the ring graph defined by the adjacency matrix A given in the `Matlab` program shown below:

```
A = diag(ones(1, 11),1);
A = A + A';
A(1, 12) = 1; A(12, 1) = 1;
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on
gplot(A, v(:, [2 3]),'o')
```

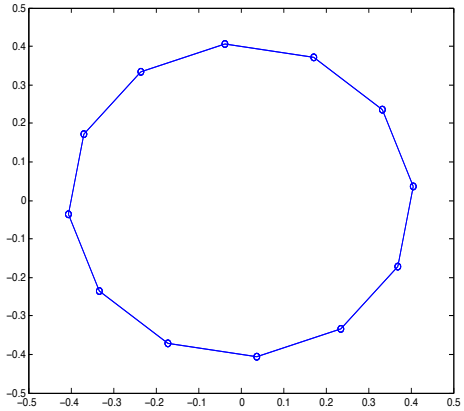

Figure 3.3: Drawing of the graph from Example 3.

Observe that we get a very nice ring; see Figure 3.3. Again $\lambda_2 = 0.2679$ is a double eigenvalue (and so are the next pairs of eigenvalues, except the last, $\lambda_{12} = 4$).

Example 4. In this example adapted from Spielman, we generate 20 randomly chosen points in the unit square, compute their Delaunay triangulation, then the adjacency matrix of the corresponding graph, and finally draw the graph using the second and third eigenvalues of the Laplacian.

```
A = zeros(20,20);
xy = rand(20, 2);
trigs = delaunay(xy(:,1), xy(:,2));
elemtrig = ones(3) - eye(3);
for i = 1:length(trigs),
 A(trigs(i,:),trigs(i,:)) = elemtrig;
end
```

```
A = double(A >0);
gplot(A,xy)
D = diag(sum(A));
L = D - A;
[v, e] = eigs(L, 3, 'sm');
figure(2)
gplot(A, v(:, [2 1]))
hold on
gplot(A, v(:, [2 1]),'o')
```

The Delaunay triangulation of the set of 20 points and the drawing of the corresponding graph are shown in Figure 3.4. The graph drawing on the right looks nicer than the graph on the left but is is no longer planar.

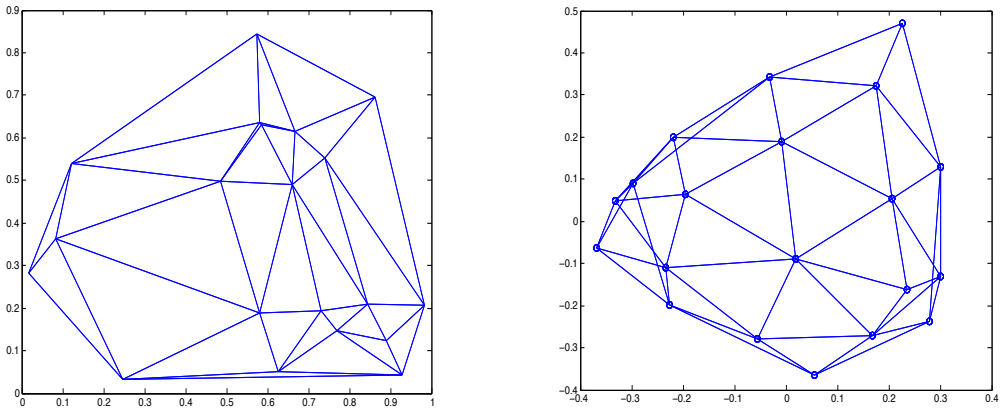

Figure 3.4: Delaunay triangulation (left) and drawing of the graph from Example 4 (right).

Example 5. Our last example, also borrowed from Spielman [21], corresponds to the skeleton of the "Buckyball," a geodesic dome invented by the architect Richard Buckminster Fuller (1895–1983). The Montréal Biosphère is an example of a geodesic dome designed by Buckminster Fuller.

```
A = full(bucky);
D = diag(sum(A));
L = D - A;
[v, e] = eig(L);
gplot(A, v(:, [2 3]))
hold on;
gplot(A,v(:, [2 3]), 'o')
```

Figure 3.5 shows a graph drawing of the Buckyball. This picture seems a bit squashed for two reasons. First, it is really a 3-dimensional graph; second, $\lambda_2 = 0.2434$ is a triple

eigenvalue. (Actually, the Laplacian of L has many multiple eigenvalues.) What we should really do is to plot this graph in $\mathbb{R}^3$ using three orthonormal eigenvectors associated with λ_2.

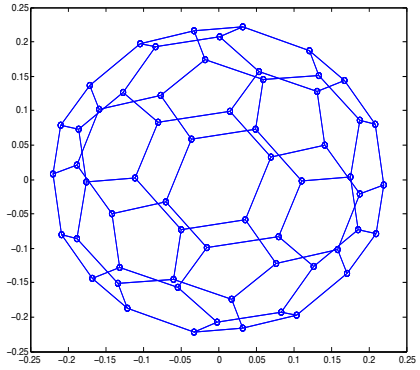

Figure 3.5: Drawing of the graph of the Buckyball.

A 3D picture of the graph of the Buckyball is produced by the following `Matlab` program, and its image is shown in Figure 3.6. It looks better!

```
[x, y] = gplot(A, v(:, [2 3]));
[x, z] = gplot(A, v(:, [2 4]));
plot3(x,y,z)
```

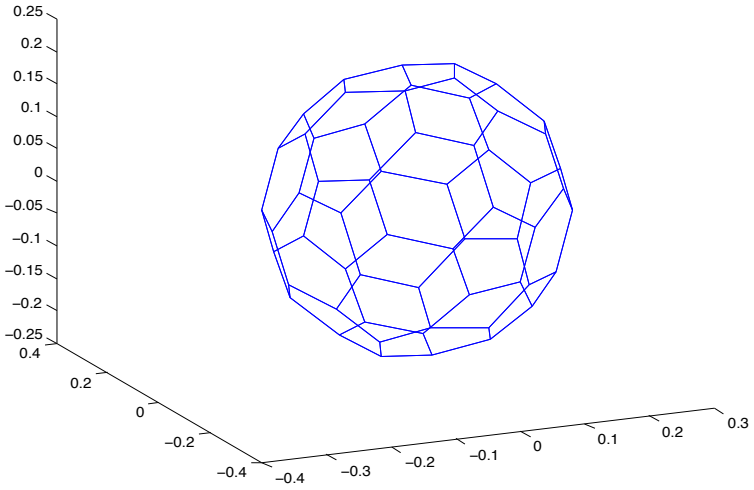

Figure 3.6: Drawing of the graph of the Buckyball in $\mathbb{R}^3$.

Chapter 4

Graph Clustering

4.1 Graph Clustering Using Normalized Cuts

Given a set of data, the goal of clustering is to partition the data into different groups according to their similarities. When the data is given in terms of a similarity graph G, where the weight $w_{i\,j}$ between two nodes v_i and v_j is a measure of similarity of v_i and v_j, the problem can be stated as follows: Find a partition $(A_1, \ldots, A_K)$ of the set of nodes V into different groups such that the edges between different groups have very low weight (which indicates that the points in different clusters are dissimilar), and the edges within a group have high weight (which indicates that points within the same cluster are similar).

The above graph clustering problem can be formalized as an optimization problem, using the notion of cut mentioned at the end of Section 2.1.

Given a subset A of the set of vertices V, recall that we define $\mathrm{cut}(A)$ by

$$\mathrm{cut}(A) = \mathrm{links}(A, \overline{A}) = \sum_{v_i \in A, v_j \in \overline{A}} w_{i\,j},$$

and that

$$\mathrm{cut}(A) = \mathrm{links}(A, \overline{A}) = \mathrm{links}(\overline{A}, A) = \mathrm{cut}(\overline{A}).$$

If we want to partition V into K clusters, we can do so by finding a partition $(A_1, \ldots, A_K)$ that minimizes the quantity

$$\mathrm{cut}(A_1, \ldots, A_K) = \frac{1}{2} \sum_{i=1}^{K} \mathrm{cut}(A_i).$$

The reason for introducing the factor $1/2$ is to avoiding counting each edge twice. In particular,

$$\mathrm{cut}(A, \overline{A}) = \mathrm{links}(A, \overline{A}).$$

For $K = 2$, the mincut problem is a classical problem that can be solved efficiently, but in practice, it does not yield satisfactory partitions. Indeed, in many cases, the mincut solution

separates one vertex from the rest of the graph. What we need is to design our cost function in such a way that it keeps the subsets A_i "reasonably large" (reasonably balanced).

A example of a weighted graph and a partition of its nodes into two clusters is shown in Figure 4.1.

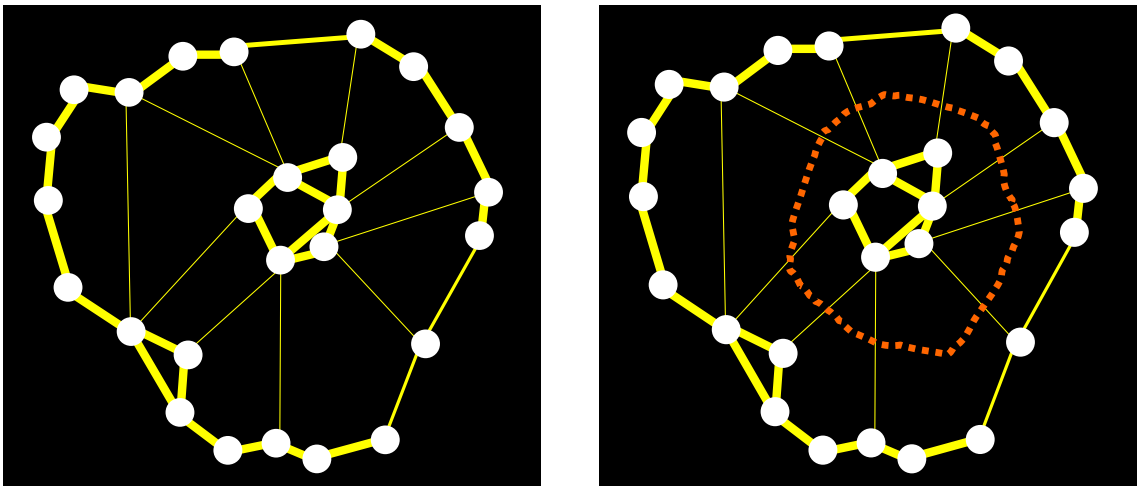

Figure 4.1: A weighted graph and its partition into two clusters.

A way to get around this problem is to normalize the cuts by dividing by some measure of each subset A_i. One possibility is to use the size (the number of elements) of A_i. Another is to use the volume $\mathrm{vol}(A_i)$ of A_i. A solution using the second measure (the volume) (for $K = 2$) was proposed and investigated in a seminal paper of Shi and Malik [20]. Subsequently, Yu (in her dissertation [23]) and Yu and Shi [24] extended the method to $K > 2$ clusters. We will describe this method later. The idea is to minimize the cost function

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{links}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)} = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_i, \overline{A_i})}{\mathrm{vol}(A_i)}.$$

We begin with the case $K = 2$, which is easier to handle.

4.2 Special Case: 2-Way Clustering Using Normalized Cuts

Our goal is to express our optimization problem in matrix form. In the case of two clusters, a single vector X can be used to describe the partition $(A_1, A_2) = (A, \overline{A})$. We need to choose the structure of this vector in such a way that $\mathrm{Ncut}(A, \overline{A})$ is equal to the Rayleigh ratio

$$\frac{X^\top L X}{X^\top D X}.$$

It is also important to pick a vector representation which is invariant under multiplication by a nonzero scalar, because the Rayleigh ratio is scale-invariant, and it is crucial to take advantage of this fact to make the denominator go away.

Let $N = |V|$ be the number of nodes in the graph G. In view of the desire for a scale-invariant representation, it is natural to assume that the vector X is of the form

$$X = (x_1, \ldots, x_N),$$

where $x_i \in \{a, b\}$ for $i = 1, \ldots, N$, for any two distinct real numbers a, b. This is an indicator vector in the sense that, for $i = 1, \ldots, N$,

$$x_i = \begin{cases} a & \text{if } v_i \in A \\ b & \text{if } v_i \notin A. \end{cases}$$

The correct interpretation is really to view X as a representative of a point in the real projective space $\mathbb{RP}^{N-1}$, namely the point $\mathbb{P}(X)$ of homogeneous coordinates $(x_1 \colon \cdots \colon x_N)$. Therefore, from now on, we view X as a vector of homogeneous coordinates representing the point $\mathbb{P}(X) \in \mathbb{RP}^{N-1}$.

Let $d = \mathbf{1}^\top D\mathbf{1}$ and $\alpha = \mathrm{vol}(A)$. Then, $\mathrm{vol}(\overline{A}) = d - \alpha$. By Proposition 2.4, we have

$$X^\top LX = (a-b)^2 \,\mathrm{cut}(A, \overline{A}),$$

and we easily check that

$$X^\top DX = \alpha a^2 + (d-\alpha)b^2.$$

Since $\mathrm{cut}(A, \overline{A}) = \mathrm{cut}(\overline{A}, A)$, we have

$$\mathrm{Ncut}(A, \overline{A}) = \frac{\mathrm{cut}(A, \overline{A})}{\mathrm{vol}(A)} + \frac{\mathrm{cut}(\overline{A}, A)}{\mathrm{vol}(\overline{A})} = \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(\overline{A})}\right) \mathrm{cut}(A, \overline{A}),$$

so we obtain

$$\mathrm{Ncut}(A, \overline{A}) = \left(\frac{1}{\alpha} + \frac{1}{d-\alpha}\right) \mathrm{cut}(A, \overline{A}) = \frac{d}{\alpha(d-\alpha)} \,\mathrm{cut}(A, \overline{A}).$$

Since

$$\frac{X^\top LX}{X^\top DX} = \frac{(a-b)^2}{\alpha a^2 + (d-\alpha)b^2} \,\mathrm{cut}(A, \overline{A}),$$

in order to have

$$\mathrm{Ncut}(A, \overline{A}) = \frac{X^\top LX}{X^\top DX},$$

we need to find a and b so that

$$\frac{(a-b)^2}{\alpha a^2 + (d-\alpha)b^2} = \frac{d}{\alpha(d-\alpha)}.$$

The above is equivalent to

$$(a-b)^2\alpha(d-\alpha) = \alpha d a^2 + (d-\alpha)db^2,$$

which can be rewritten as

$$a^2(\alpha d - \alpha(d-\alpha)) + b^2(d^2 - \alpha d - \alpha(d-\alpha)) + 2\alpha(d-\alpha)ab = 0.$$

The above yields

$$a^2\alpha^2 + b^2(d^2 - 2\alpha d + \alpha^2) + 2\alpha(d-\alpha)ab = 0,$$

that is,

$$a^2\alpha^2 + b^2(d-\alpha)^2 + 2\alpha(d-\alpha)ab = 0,$$

which reduces to

$$(a\alpha + b(d-\alpha))^2 = 0.$$

Therefore, we get the condition

$$a\alpha + b(d-\alpha) = 0. \tag{$\dagger$}$$

Note that condition (†) applied to a vector X whose components are a or b is equivalent to the fact that X is orthogonal to $D\mathbf{1}$, since

$$X^\top D\mathbf{1} = \alpha a + (d-\alpha)b,$$

where $\alpha = \mathrm{vol}(\{v_i \in V \mid x_i = a\})$.

We claim the following two facts. For any nonzero vector X whose components are a or b, if $X^\top D\mathbf{1} = \alpha a + (d-\alpha)b = 0$, then

(1) $\alpha \neq 0$ and $\alpha \neq d$ iff $a \neq 0$ and $b \neq 0$.

(2) if $a, b \neq 0$, then $a \neq b$.

(1) First assume that $a \neq 0$ and $b \neq 0$. If $\alpha = 0$, then $\alpha a + (d-\alpha)b = 0$ yields $db = 0$ with $d \neq 0$, which implies $b = 0$, a contradiction. If $d - \alpha = 0$, then we get $da = 0$ with $d \neq 0$, which implies $a = 0$, a contradiction.

Conversely, assume that $\alpha \neq 0$ and $\alpha \neq d$. If $a = 0$, then from $\alpha a + (d-\alpha)b = 0$ we get $(d-\alpha)b = 0$, which implies $b = 0$, contradicting the fact that $X \neq 0$. Similarly, if $b = 0$, then we get $\alpha a = 0$, which implies $a = 0$, contradicting the fact that $X \neq 0$.

(2) If $a, b \neq 0$, $a = b$ and $\alpha a + (d-\alpha)b = 0$, then $\alpha a + (d-\alpha)a = 0$, and since $a \neq 0$, we deduce that $d = 0$, a contradiction.

If $X^\top D\mathbf{1} = \alpha a + (d-\alpha)b = 0$ and $a, b \neq 0$, then

$$b = -\frac{\alpha}{(d-\alpha)}\, a,$$

so we get

$$\begin{aligned}\alpha a^2 + (d-\alpha)b^2 &= \alpha\frac{(d-\alpha)^2}{\alpha^2}b^2 + (d-\alpha)b^2 \\ &= (d-\alpha)\left(\frac{d-\alpha}{\alpha}+1\right)b^2 = \frac{(d-\alpha)db^2}{\alpha},\end{aligned}$$

and

$$\begin{aligned}(a-b)^2 &= \left(-\frac{(d-\alpha)}{\alpha}\,b - b\right)^2 \\ &= \left(\frac{d-\alpha}{\alpha}+1\right)^2 b^2 = \frac{d^2b^2}{\alpha^2}.\end{aligned}$$

Since

$$\begin{aligned}X^\top DX &= \alpha a^2 + (d-\alpha)b^2 \\ X^\top LX &= (a-b)^2\,\mathrm{cut}(A,\overline{A}),\end{aligned}$$

we obtain

$$\begin{aligned}X^\top DX &= \frac{(d-\alpha)db^2}{\alpha} = \frac{\alpha da^2}{(d-\alpha)} \\ X^\top LX &= \frac{d^2b^2}{\alpha^2}\,\mathrm{cut}(A,\overline{A}) = \frac{d^2a^2}{(d-\alpha)^2}\,\mathrm{cut}(A,\overline{A}).\end{aligned}$$

If we wish to make α disappear, we pick

$$a = \sqrt{\frac{d-\alpha}{\alpha}}, \quad b = -\sqrt{\frac{\alpha}{d-\alpha}},$$

and then

$$\begin{aligned}X^\top DX &= d \\ X^\top LX &= \frac{d^2}{\alpha(d-\alpha)}\,\mathrm{cut}(A,\overline{A}) = d\,\mathrm{Ncut}(A,\overline{A}).\end{aligned}$$

In this case, we are considering indicator vectors of the form

$$\left\{(x_1,\ldots,x_N) \mid x_i \in \left\{\sqrt{\frac{d-\alpha}{\alpha}}, -\sqrt{\frac{\alpha}{d-\alpha}}\right\}, \alpha = \mathrm{vol}(A)\right\},$$

for any nonempty proper subset A of V. This is the choice adopted in von Luxburg [22]. Shi and Malik [20] use

$$a = 1, \quad b = -\frac{\alpha}{d-\alpha} = -\frac{k}{1-k},$$

with

$$k = \frac{\alpha}{d}.$$

Another choice found in the literature (for example, in Belkin and Niyogi [2]) is

$$a = \frac{1}{\alpha}, \quad b = -\frac{1}{d-\alpha}.$$

However, there is no need to restrict solutions to be of either of these forms. So, let

$$\mathcal{X} = \big\{(x_1, \ldots, x_N) \mid x_i \in \{a, b\},\ a, b \in \mathbb{R},\ a, b \neq 0\big\},$$

so that our solution set is

$$\mathcal{K} = \big\{X \in \mathcal{X} \mid X^\top D\mathbf{1} = 0\big\},$$

because by previous observations, since vectors $X \in \mathcal{X}$ have nonzero components, $X^\top D\mathbf{1} = 0$ implies that $\alpha \neq 0$, $\alpha \neq d$, and $a \neq b$, where $\alpha = \mathrm{vol}(\{v_i \in V \mid x_i = a\})$. Actually, to be perfectly rigorous, we are looking for solutions in $\mathbb{RP}^{N-1}$, so our solution set is really

$$\mathbb{P}(\mathcal{K}) = \big\{(x_1 \colon \cdots \colon x_N) \in \mathbb{RP}^{N-1} \mid (x_1, \ldots, x_N) \in \mathcal{K}\big\}.$$

Consequently, our minimization problem can be stated as follows:

Problem PNC1

$$\begin{array}{lll} \text{minimize} & \dfrac{X^\top LX}{X^\top DX} & \\ \text{subject to} & X^\top D\mathbf{1} = 0, & X \in \mathcal{X}. \end{array}$$

It is understood that the solutions are points $\mathbb{P}(X)$ in $\mathbb{RP}^{N-1}$.

Since the Rayleigh ratio and the constraints $X^\top D\mathbf{1} = 0$ and $X \in \mathcal{X}$ are scale-invariant (for any $\lambda \neq 0$, the Rayleigh ratio does not change if X is replaced by λX, $X \in \mathcal{X}$ iff $\lambda X \in \mathcal{X}$, and $(\lambda X)^\top D\mathbf{1} = \lambda X^\top D\mathbf{1} = 0$), we are led to the following formulation of our problem:

Problem PNC2

$$\begin{array}{lllll} \text{minimize} & X^\top LX & & & \\ \text{subject to} & X^\top DX = 1, & X^\top D\mathbf{1} = 0, & & X \in \mathcal{X}. \end{array}$$

Because problem PNC2 requires the constraint $X^\top DX = 1$ to be satisfied, it does not have the same set of solutions as problem PNC1. Nevertheless, problem PNC2 is equivalent to problem PNC1, in the sense that if X is any minimal solution of PNC1, then $X/(X^\top DX)^{1/2}$ is a minimal solution of PNC2 (with the same minimal value for the objective functions), and if X is a minimal solution of PNC2, then λX is a minimal solution for PNC1 for all $\lambda \neq 0$ (with the same minimal value for the objective functions). Equivalently,

problems PNC1 and PNC2 have the same set of minimal solutions as points $\mathbb{P}(X) \in \mathbb{RP}^{N-1}$ given by their homogeneous coordinates X.

Unfortunately, this is an NP-complete problem, as shown by Shi and Malik [20]. As often with hard combinatorial problems, we can look for a *relaxation* of our problem, which means looking for an optimum in a larger continuous domain. After doing this, the problem is to find a discrete solution which is close to a continuous optimum of the relaxed problem.

The natural relaxation of this problem is to allow X to be any nonzero vector in $\mathbb{R}^N$, and we get the problem:

$$\text{minimize} \quad X^\top LX \quad \text{subject to} \quad X^\top DX = 1, \quad X^\top D\mathbf{1} = 0.$$

In order to apply Proposition A.2, we make the change of variable $Y = D^{1/2}X$, so that $X = D^{-1/2}Y$. Then, the condition $X^\top DX = 1$ becomes

$$Y^\top Y = 1,$$

the condition

$$X^\top D\mathbf{1} = 0$$

becomes

$$Y^\top D^{1/2}\mathbf{1} = 0,$$

and

$$X^\top LX = Y^\top D^{-1/2}LD^{-1/2}Y.$$

We obtain the problem:

$$\text{minimize} \quad Y^\top D^{-1/2}LD^{-1/2}Y \quad \text{subject to} \quad Y^\top Y = 1, \quad Y^\top D^{1/2}\mathbf{1} = 0.$$

Because $L\mathbf{1} = 0$, the vector $D^{1/2}\mathbf{1}$ belongs to the nullspace of the symmetric Laplacian $L_{\text{sym}} = D^{-1/2}LD^{-1/2}$. By Proposition A.2, minima are achieved by any unit eigenvector Y of the second eigenvalue $\nu_2 > 0$ of L_{sym}. Since 0 is the smallest eigenvalue of L_{sym} and since $D^{1/2}\mathbf{1}$ belongs to the nullspace of L_{sym}, as the eigenvectors associated with distinct eigenvalues are orthogonal, the vector Y is orthogonal to $D^{1/2}\mathbf{1}$, so the constraint $Y^\top D^{1/2}\mathbf{1} = 0$ is satisfied. Then, $Z = D^{-1/2}Y$ is a solution of our original relaxed problem. Note that because Z is nonzero and orthogonal to $D\mathbf{1}$, a vector with positive entries, it must have negative and positive entries.

The next question is to figure how close is Z to an exact solution in $\mathcal{X}$. Actually, because solutions are points in $\mathbb{RP}^{N-1}$, the correct statement of the question is: Find an exact solution $\mathbb{P}(X) \in \mathbb{P}(\mathcal{X})$ which is the closest (in a suitable sense) to the approximate solution $\mathbb{P}(Z) \in \mathbb{RP}^{N-1}$. However, because $\mathcal{X}$ is closed under the antipodal map, as explained in Appendix B, minimizing the distance $d(\mathbb{P}(X), \mathbb{P}(Z))$ on $\mathbb{RP}^{N-1}$ is equivalent to minimizing the Euclidean distance $\|X - Z\|_2$, where X and Z are representatives of $\mathbb{P}(X)$ and $\mathbb{P}(Z)$ on

the unit sphere (if we use the Riemannian metric on $\mathbb{RP}^{N-1}$ induced by the Euclidean metric on $\mathbb{R}^N$).

We may assume $b < 0$, in which case $a > 0$. If all entries in Z are nonzero, due to the projective nature of the solution set, it seems reasonable to say that the partition of V is defined by the signs of the entries in Z. Thus, A will consist of nodes those v_i for which $x_i > 0$. Elements corresponding to zero entries can be assigned to either A or $\overline{A}$, unless additional information is available. In our implementation, they are assigned to A.

Here are some examples of normalized cuts found by a fairly naive implementation of the method. The weight matrix of the first example is

$$W_1 = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \end{pmatrix}.$$

Its underlying graph has 9 nodes and 9 edges and is shown in Figure 4.2 on the left. The normalized cut found by the algorithm is shown in the middle; the edge of the cut is shown in magenta, and the vertices of the blocks of the partition are shown in blue and red. The figure on the right shows the two disjoint subgraphs obtained after deleting the cut edge.

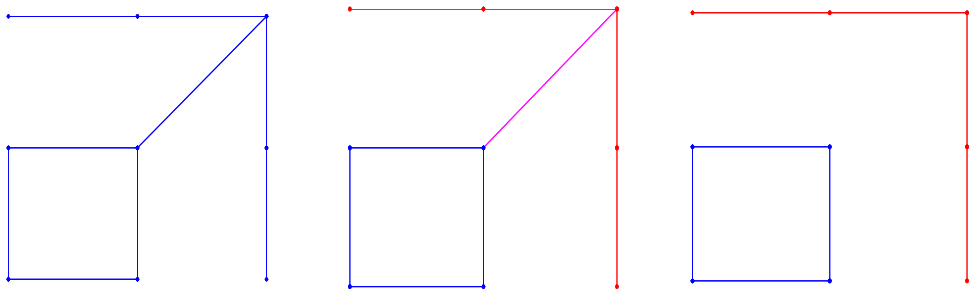

Figure 4.2: Underlying graph of the matrix W_1 (left); normalized cut (middle); blocks of the cut (right).

The weight matrix of the second example is

$$W_2 = \begin{pmatrix} 0 & 3 & 6 & 3 \\ 3 & 0 & 0 & 3 \\ 6 & 0 & 0 & 3 \\ 3 & 3 & 3 & 0 \end{pmatrix}.$$

Its underlying graph has 4 nodes and 5 edges and is shown in Figure 4.3 on the left. The normalized cut found by the algorithm is shown in the middle; the edges of the cut are shown in magenta, and the vertices of the blocks of the partition are shown in blue and red. The figure on the right shows the two disjoint subgraphs obtained after deleting the cut edges.

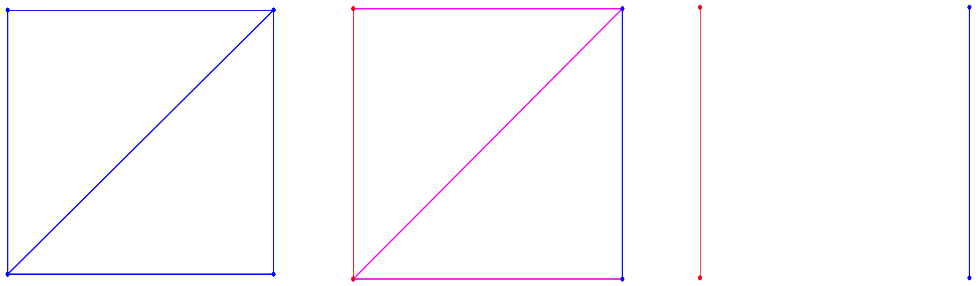

Figure 4.3: Underlying graph of the matrix W_2 (left); normalized cut (middle); blocks of the cut (right).

The weight matrix W_3 of the third example is the adjacency matrix of the complete graph on 12 vertices. All nondiagonal entries are equal to 1, and the diagonal entries are equal to 0. This graph has 66 edges and is shown in Figure 4.4 on the left.

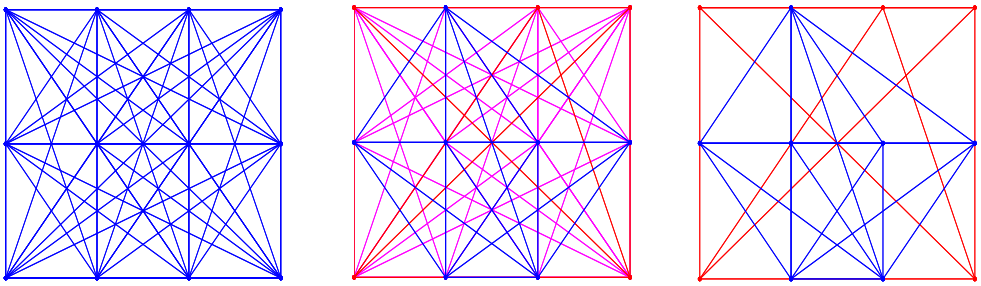

Figure 4.4: Underlying graph of the matrix W_3 (left); normalized cut (middle); blocks of the cut (right).

The normalized cut found by the algorithm is shown in the middle; the edges of the cut are shown in magenta, and the vertices of the blocks of the partition are shown in blue and red. The figure on the right shows the two disjoint subgraphs obtained after deleting the cut edges. Recall that $L_{\text{sym}} = B_3 B_3^\top$ for any incidence matrix B_3 associated with W_3, so that for any SVD $U_3 \Sigma_3 V_3$ of B_3, the vectors in U_3 are eigenvectors of L_{sym} for its eigenvalues listed in decreasing order. The normalized Laplacian of this weight matrix has the eigenvalue 1.0909 with multiplicity 11 (and any incidence matrix B_3 associated with W_3 has the singular value 1.0445 with multiplicity 11). Computing the SVD $U_3 \Sigma_3 V_3$ of B_3 and picking the next to the last eigenvector in U_3 yields a partition consisting of 7 and 5 nodes. There are other

eigenvectors that yield partitions with an equal number of elements. Since a complete graph has a lot of symmetries, it is not surprising that there are many different solutions. In fact, examination of the eigenvectors of U_3 reveal very unbalanced solutions.

For graphs where the number N of edges is very large and the number of edges is $O(N^2)$, computing the SVD of the incidence matrix B is not practical. Instead, we compute an SVD for L_{sym}, which appears to be more stable that diagonalizing L_{sym}.

Our naive algorithm treated zero as a positive entry. Now, using the fact that

$$b = -\frac{\alpha a}{d - \alpha},$$

a better solution is to look for a vector $X \in \mathbb{R}^N$ with $X_i \in \{a, b\}$ which is closest to a minimum Z of the relaxed problem (in the sense that $\|X - Z\|$ is minimized) and with $\|X\| = \|Z\|$. We designed the following algorithm.

A vector X describing a partition $(A, \overline{A})$ is of the form

$$X_i = \begin{cases} a & \text{if } v_i \in A \\ -\beta a & \text{otherwise,} \end{cases}$$

with

$$\alpha = \text{vol}(\{v_i \mid v_i \in A\}), \qquad \beta = \frac{\alpha}{d - \alpha},$$

and where $a > 0$ is chosen so that $\left\|\overline{X}\right\| = \|Z\|$. For any solution Z of the relaxed problem, let $I_Z^+ = \{i \mid Z_i > 0\}$ be the set of indices of positive entries in Z, $I_Z^- = \{i \mid Z_i < 0\}$ the set of indices of negative entries in Z, $I_Z^0 = \{i \mid Z_i = 0\}$ the set of indices of zero entries in Z. Initially, it makes sense to form a discrete approximation $\overline{X}$ of Z such that all entries of index in I_Z^+ are assigned the value $a > 0$ (to be determined later), and all other entries are assigned the value $-\beta a$. In order for $\overline{X}$ and Z to have the same norm, since

$$\left\|\overline{X}\right\|^2 = (n_a + \beta^2(N - n_a))a^2$$

with

$$n_a = |I_Z^+|, \qquad \alpha = \text{vol}(\{v_i \mid i \in I_Z^+\}), \qquad \beta = \frac{\alpha}{d - \alpha},$$

we set

$$a = \frac{\|Z\|}{\sqrt{(n_a + \beta^2(N - n_a))}}.$$

The problems is to determine whether an entry with an index $i \in I_Z^0$ (which is initially assigned the value $-\beta a$) should be reassigned the value a. To make the decision, we form the new discrete solution $\widetilde{X}$ obtained from $\overline{X}$ by adding the index i to I_Z^+, and updating

α, β and a; this is done in step (2). Then, we compare $\|\overline{X} - Z\|$ and $\|\widetilde{X} - Z\|$ and keep the vector that yields the smallest norm. We delete i from I_Z^0, and repeat step (2). After a finite number of steps, I_Z^0 becomes empty and we obtain a discrete solution $\overline{X}$ which is typically closer to X than the starting approximate solution.

We also need to decide whether to start with Z or $-Z$ (remember that solution are determined up to a nonzero scalar). We proceed as follows. Let Z^+ and Z^- be the vectors given by

$$Z_i^+ = \begin{cases} Z_i & \text{if } i \in I_Z^+ \\ 0 & \text{if } i \notin I_Z^+ \end{cases} \qquad\qquad Z_i^- = \begin{cases} Z_i & \text{if } i \in I_Z^- \\ 0 & \text{if } i \notin I_Z^- \end{cases}.$$

Also let $n_a = |I_Z^+|$, $n_b = |I_Z^-|$, let $\overline{a}$ and $\overline{b}$ be the average of the positive and negative entries in Z respectively, that is,

$$\overline{a} = \frac{\sum_{i \in I_Z^+} Z_i}{n_a} \qquad\qquad \overline{b} = \frac{\sum_{i \in I_Z^-} Z_i}{n_b},$$

and let $\overline{Z^+}$ and $\overline{Z^-}$ be the vectors given by

$$(\overline{Z^+})_i = \begin{cases} \overline{a} & \text{if } i \in I_Z^+ \\ 0 & \text{if } i \notin I_Z^+ \end{cases} \qquad\qquad (\overline{Z^-})_i = \begin{cases} \overline{b} & \text{if } i \in I_Z^- \\ 0 & \text{if } i \notin I_Z^- \end{cases}.$$

If $\left\|\overline{Z^+} - Z^+\right\| > \left\|\overline{Z^-} - Z^-\right\|$, then replace Z by $-Z$.

Step 1 of the algorithm is to compute an initial approximate discrete solution $\overline{X}$.

(1) Let

$$n_a = |I_Z^+|, \qquad\qquad \alpha = \mathrm{vol}(\{v_i \mid i \in I_Z^+\}), \qquad\qquad \beta = \frac{\alpha}{d - \alpha},$$

and form the vector $\overline{X}$ with

$$\overline{X}_i = \begin{cases} a & \text{if } i \in I_Z^+ \\ -\beta a & \text{otherwise,} \end{cases}$$

such that $\left\|\overline{X}\right\| = \|Z\|$, where the scalar a is determined by

$$a = \frac{\|Z\|}{\sqrt{(n_a + \beta^2(N - n_a))}}.$$

Next, pick some entry with index $i \in I_Z^0$ and see whether we can impove the solution $\overline{X}$ by adding i to I_Z^+.

(2) While $I_Z^0 \neq \emptyset$, pick the smallest index $i \in I_Z^0$, compute

$$\begin{aligned}\widetilde{I}_Z^+ &= I_Z^+ \cup \{i\}\\ \widetilde{n}_a &= n_a + 1\\ \widetilde{\alpha} &= \alpha + d(v_i)\\ \widetilde{\beta} &= \frac{\widetilde{\alpha}}{d - \widetilde{\alpha}},\end{aligned}$$

and then $\widetilde{X}$ with

$$\widetilde{X}_j = \begin{cases}\widetilde{a} & \text{if } j \in \widetilde{I}_Z^+\\ -\widetilde{\beta}\widetilde{a} & \text{otherwise,}\end{cases}$$

and

$$\widetilde{a} = \frac{\|Z\|}{\sqrt{\widetilde{n}_a + \widetilde{\beta}^2(N - \widetilde{n}_a)}}.$$

Set $I_Z^0 = I_Z^0 - \{i\}$. If $\|\widetilde{X} - Z\| < \|\overline{X} - Z\|$, then let $\overline{X} = \widetilde{X}$, $I_Z^+ = \widetilde{I}_Z^+$, $n_a = \widetilde{n}_a$, $\alpha = \widetilde{\alpha}$. Go back to (2).

(3) The final answer if $\overline{X}$.

I implemented this algorithm, and it seems to do a god job dealing with zero entries in the continuous solution Z.

4.3 K-Way Clustering Using Normalized Cuts

We now consider the general case in which $K \geq 3$. Two crucial issues need to be addressed (to the best of our knowledge, these points are not clearly articulated in the literature).

1. The choice of a matrix representation for partitions on the set of vertices. It is important that such a representation be scale-invariant. It is also necessary to state necessary and sufficient conditions for such matrices to represent a partition.

2. The choice of a metric to compare solutions. It turns out that the space of discrete solutions can be viewed as a subset of the K-fold product $(\mathbb{RP}^{N-1})^K$ of the projective space $\mathbb{RP}^{N-1}$. Version 1 of the formulation of our minimization problem (PNC1) makes this point clear. However, the relaxation $(*_2)$ of version 2 of our minimization problem (PNC2), which is equivalent to version 1, reveals that that the solutions of the relaxed problem $(*_2)$ are members of the *Grassmannian* $G(K, N)$. Thus, we have two choices of metrics: (1) a metric on $(\mathbb{RP}^{N-1})^K$; (2) a metric on $G(K, N)$. We discuss the first choice, which is the choice implicitly adopted by Shi and Yu. Actually, it appears that it is difficult to deal with the product metric on $(\mathbb{RP}^{N-1})^K$ induced by a metric on $\mathbb{RP}^{N-1}$. Instead, we approximate a metric on $(\mathbb{RP}^{N-1})^K$ using the Frobenius norm; see Section 4.5 for details.

We describe a partition $(A_1, \ldots, A_K)$ of the set of nodes V by an $N \times K$ matrix $X = [X^1 \cdots X^K]$ whose columns $X^1, \ldots, X^K$ are indicator vectors of the partition $(A_1, \ldots, A_K)$. Inspired by what we did in Section 4.2, we assume that the vector X^j is of the form

$$X^j = (x_1^j, \ldots, x_N^j),$$

where $x_i^j \in \{a_j, b_j\}$ for $j = 1, \ldots, K$ and $i = 1, \ldots, N$, and where a_j, b_j are any two distinct real numbers. The vector X^j is an indicator vector for A_j in the sense that, for $i = 1, \ldots, N$,

$$x_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ b_j & \text{if } v_i \notin A_j. \end{cases}$$

When $\{a_j, b_j\} = \{0, 1\}$ for $j = 1, \ldots, K$, such a matrix is called a *partition matrix* by Yu and Shi. However, such a choice is premature, since it is better to have a scale-invariant representation to make the denominators of the Rayleigh ratios go away.

Since the partition $(A_1, \ldots, A_K)$ consists of nonempty pairwise disjoint blocks whose union is V, some conditions on X are required to reflect these properties, but we will worry about this later.

As in Section 4.2, we seek conditions on the a_js and the b_js in order to express the normalized cut $\mathrm{Ncut}(A_1, \ldots, A_K)$ as a sum of Rayleigh ratios. Then, we reformulate our optimization problem in a more convenient form, by chasing the denominators in the Rayleigh ratios, and by expressing the objective function in terms of the *trace* of a certain matrix. This will reveal the important fact that the solutions of the relaxed problem are right-invariant under multiplication by a $K \times K$ orthogonal matrix.

Let $d = \mathbf{1}^\top D \mathbf{1}$ and $\alpha_j = \mathrm{vol}(A_j)$, so that $\alpha_1 + \cdots + \alpha_K = d$. Then, $\mathrm{vol}(\overline{A_j}) = d - \alpha_j$, and as in Section 4.2, we have

$$\begin{aligned} (X^j)^\top L X^j &= (a_j - b_j)^2 \,\mathrm{cut}(A_j, \overline{A_j}), \\ (X^j)^\top D X^j &= \alpha_j a_j^2 + (d - \alpha_j) b_j^2. \end{aligned}$$

When $K \geq 3$, unlike the case $K = 2$, in general we have $\mathrm{cut}(A_j, \overline{A_j}) \neq \mathrm{cut}(A_k, \overline{A_k})$ if $j \neq k$, and since

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)},$$

we would like to choose a_j, b_j so that

$$\frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)} = \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \quad j = 1, \ldots, K,$$

because this implies that

$$\mu(X) = \mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)} = \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j}.$$

Since

$$\frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} = \frac{(a_j - b_j)^2 \operatorname{cut}(A_j, \overline{A_j})}{\alpha_j a_j^2 + (d - \alpha_j) b_j^2}$$

and $\operatorname{vol}(A_j) = \alpha_j$, in order to have

$$\frac{\operatorname{cut}(A_j, \overline{A_j})}{\operatorname{vol}(A_j)} = \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \quad j = 1, \ldots, K,$$

we need to have

$$\frac{(a_j - b_j)^2}{\alpha_j a_j^2 + (d - \alpha_j) b_j^2} = \frac{1}{\alpha_j} \quad j = 1, \ldots, K.$$

Thus, we must have

$$(a_j^2 - 2a_j b_j + b_j^2)\alpha_j = \alpha_j a_j^2 + (d - \alpha_j) b_j^2,$$

which yields

$$2\alpha_j b_j (b_j - a_j) = d b_j^2.$$

The above equation is trivially satisfied if $b_j = 0$. If $b_j \neq 0$, then

$$2\alpha_j (b_j - a_j) = d b_j,$$

which yields

$$a_j = \frac{2\alpha_j - d}{2\alpha_j} b_j.$$

This choice seems more complicated that the choice $b_j = 0$, so we will opt for the choice $b_j = 0$, $j = 1, \ldots, K$. With this choice, we get

$$(X^j)^\top D X^j = \alpha_j a_j^2.$$

Thus, it makes sense to pick

$$a_j = \frac{1}{\sqrt{\alpha_j}} = \frac{1}{\sqrt{\operatorname{vol}(A_j)}}, \quad j = 1, \ldots, K,$$

which is the solution presented in von Luxburg [22]. This choice also corresponds to the scaled partition matrix used in Yu [23] and Yu and Shi [24].

When $N = 10$ and $K = 4$, an example of a matrix X representing the partition of $V = \{v_1, v_2, \ldots, v_{10}\}$ into the four blocks

$$\{A_1, A_2, A_3, A_4\} = \{\{v_2, v_4, v_6\}, \{v_1, v_5\}, \{v_3, v_8, v_{10}\}, \{v_7, v_9\}\},$$

is shown below:

$$X = \begin{pmatrix} 0 & a_2 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_4 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \\ 0 & 0 & a_3 & 0 \end{pmatrix}.$$

Let us now consider the problem of finding necessary and sufficient conditions for a matrix X to represent a partition of V.

When $b_j = 0$, the pairwise disjointness of the A_i is captured by the orthogonality of the X^i:

$$(X^i)^\top X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j. \tag{$*$}$$

This is because, for any matrix X where the nonzero entries in each column have the same sign, for any $i \neq j$, the condition

$$(X^i)^\top X^j = 0$$

says that for every $k = 1, \ldots, N$, if $x_k^i \neq 0$ then $x_k^j = 0$.

When we formulate our minimization problem in terms of Rayleigh ratios, conditions on the quantities $(X^i)^\top D X^i$ show up, and it is more convenient to express the orthogonality conditions using the quantities $(X^i)^\top D X^j$ instead of the $(X^i)^\top X^j$, because these various conditions can be combined into a single condition involving the matrix $X^\top D X$. Now, because D is a diagonal matrix with positive entries and because the nonzero entries in each column of X have the same sign, for any $i \neq j$, the condition

$$(X^i)^\top X^j = 0$$

is equivalent to

$$(X^i)^\top D X^j = 0, \tag{$**$}$$

since, as above, it means that for $k = 1, \ldots, N$, if $x_k^i \neq 0$ then $x_k^j = 0$. Observe that the orthogonality conditions $(*)$ (and $(**)$) are equivalent to the fact that every row of X has at most one nonzero entry.

Remark: The disjointness condition

$$X\mathbf{1}_K = \mathbf{1}_N$$

is used in Yu [23]. However, this condition does guarantee the disjointness of the blocks. For example, it is satisfied by the matrix X whose first column is $\mathbf{1}_N$, with 0 everywhere else.

Each A_j is nonempty iff $X^j \neq 0$, and the fact that the union of the A_j is V is captured by the fact that each row of X must have some nonzero entry (every vertex appears in some block). It is not immediately obvious how to state conveniently this condition in matrix form.

Observe that the diagonal entries of the matrix $XX^\top$ are the square Euclidean norms of the rows of X. Therefore, we can assert that these entries are all nonzero. Let DIAG be the function which returns the diagonal matrix (containing the diagonal of A),

$$\mathrm{DIAG}(A) = \mathrm{diag}(a_{1\,1}, \ldots, a_{n\,n}),$$

for any square matrix $A = (a_{i\,j})$. Then, the condition for the rows of X to be nonzero can be stated as

$$\det(\mathrm{DIAG}(XX^\top)) \neq 0.$$

Since every row of any matrix X representing a partition has a single nonzero entry a_j, we have

$$X^\top X = \mathrm{diag}\left(n_1 a_1^2, \ldots, n_K a_K^2\right),$$

where n_j is the number of elements in A_j, the jth block of the partition. Therefore, an equivalent condition for the columns of X to be nonzero is

$$\det(X^\top X) \neq 0.$$

Remark: The matrix

$$\mathrm{DIAG}(XX^\top)^{-1/2} X$$

is the result of normalizing the rows of X so that they have Euclidean norm 1. This normalization step is used by Yu [23] in the search for a discrete solution closest to a solution of a relaxation of our original problem. For our special matrices representing partitions, normalizing the rows will have the effect of rescaling the columns (if row i has a_j in column j, then all nonzero entries in column j are equal to a_j), but for a more general matrix, this is false. Thus, in general, $\mathrm{DIAG}(XX^\top)^{-1/2} X$ is not a solution of the original problem. Still, as we will see in Section 4.5, this matrix is a pretty good approximation to a discrete solution.

Another condition which does not involve explicitly a determinant and is scale-invariant stems from the observation that not only

$$X^\top X = \mathrm{diag}\left(n_1 a_1^2, \ldots, n_K a_K^2\right),$$

but

$$X^\top \mathbf{1}_N = \begin{pmatrix} n_1 a_1 \\ \vdots \\ n_K a_K \end{pmatrix},$$

and these equations imply that

$$(X^\top X)^{-1}X^\top \mathbf{1}_N = \begin{pmatrix} \frac{1}{a_1} \\ \vdots \\ \frac{1}{a_K} \end{pmatrix},$$

and thus

$$X(X^\top X)^{-1}X^\top \mathbf{1}_N = \mathbf{1}_N. \tag{\dagger}$$

When $a_j = 1$ for $j = 1, \ldots, K$, we have $(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1}_K$, and condition (†) reduces to

$$X\mathbf{1}_K = \mathbf{1}_N.$$

Note that because the columns of X are linearly independent, $(X^\top X)^{-1}X^\top$ is the pseudo-inverse X^+ of X. Consequently, if $X^\top X$ is invertible, condition (†) can also be written as

$$XX^+\mathbf{1}_N = \mathbf{1}_N.$$

However, it is well known that XX^+ is the orthogonal projection of $\mathbb{R}^K$ onto the range of X (see Gallier [8], Section 14.1), so the condition $XX^+\mathbf{1}_N = \mathbf{1}_N$ is equivalent to the fact that $\mathbf{1}_N$ belongs to the range of X. In retrospect, this should have been obvious since the columns of a solution X satisfy the equation

$$a_1^{-1}X^1 + \cdots + a_K^{-1}X^K = \mathbf{1}_N.$$

We emphasize that it is important to use conditions that are invariant under multiplication by a nonzero scalar, because the Rayleigh ratio is scale-invariant, and it is crucial to take advantage of this fact to make the denominators go away.

If we let

$$\mathcal{X} = \Big\{[X^1 \ \ldots \ X^K] \mid X^j = a_j(x_1^j, \ldots, x_N^j),\ x_i^j \in \{1, 0\}, a_j \in \mathbb{R},\ X^j \neq 0\Big\}$$

(note that the condition $X^j \neq 0$ implies that $a_j \neq 0$), then the set of matrices representing partitions of V into K blocks is

$$\begin{aligned} \mathcal{K} = \Big\{X = [X^1 \ \cdots \ X^K] \quad \mid \quad & X \in \mathcal{X}, \\ & (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1}\Big\}. \end{aligned}$$

Since for matrices in $\mathcal{K}$, the orthogonality conditions $(X^i)^\top D X^j = 0$ are equivalent to the orthogonality conditions $(X^i)^\top X^j = 0$, and since matrices in $\mathcal{X}$ have nonzero columns, $X^\top X$ is invertible, so the last condition makes sense.

As in the case $K = 2$, to be rigorous, the solution are really K-tuples of points in $\mathbb{RP}^{N-1}$, so our solution set is really

$$\mathbb{P}(\mathcal{K}) = \Big\{(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)) \mid [X^1 \ \cdots \ X^K] \in \mathcal{K}\Big\}.$$

In view of the above, we have our first formulation of K-way clustering of a graph using normalized cuts, called problem PNC1 (the notation PNCX is used in Yu [23], Section 2.1):

K-way Clustering of a graph using Normalized Cut, Version 1: Problem PNC1

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \\ \text{subject to} & (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}, \qquad\qquad X \in \mathcal{X}. \end{array}$$

As in the case $K = 2$, the solutions that we are seeking are K-tuples $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K))$ of points in $\mathbb{RP}^{N-1}$ determined by their homogeneous coordinates $X^1, \ldots, X^K$.

Remark: Because

$$(X^j)^\top L X^j = (X^j)^\top D X^j - (X^j)^\top W X^j = \mathrm{vol}(A_j) - (X^j)^\top W X^j,$$

Instead of minimizing

$$\mu(X^1, \ldots, X^K) = \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j},$$

we can maximize

$$\epsilon(X^1, \ldots, X^K) = \sum_{j=1}^{K} \frac{(X^j)^\top W X^j}{(X^j)^\top D X^j},$$

since

$$\epsilon(X^1, \ldots, X^K) = K - \mu(X^1, \ldots, X^K).$$

This second option is the one chosen by Yu [23] and Yu and Shi [24] (actually, they work with $\frac{1}{K}(K - \mu(X^1, \ldots, X^K))$, but this doesn't make any difference). Theoretically, minimizing $\mu(X^1, \ldots, X^K)$ is equivalent to maximizing $\epsilon(X^1, \ldots, X^K)$, but from a practical point of view, it is preferable to maximize $\epsilon(X^1, \ldots, X^K)$. This is because minimizing solutions of μ are obtained from (unit) eigenvectors corresponding to the K *smallest* eigenvalues of $L_{\mathrm{sym}} = D^{-1/2} L D^{-1/2}$ (by multiplying these eigenvectors by $D^{1/2}$). However, numerical methods for computing eigenvalues and eigenvectors of a symmetric matrix do much better at computing largest eigenvalues. Since $L_{\mathrm{sym}} = I - D^{-1/2} W D^{-1/2}$, the eigenvalues of L_{sym}

listed in increasing order correspond to the eigenvalues of $I - L_{\text{sym}} = D^{-1/2}WD^{-1/2}$ listed in decreasing order. Furthermore, v is an eigenvector of L_{sym} for the ith smallest eigenvalue ν_i iff v is an eigenvector of $I - L_{\text{sym}}$ for the $(N+1-i)$th largest eigenvalue ν_i. Therefore, it is preferable to find the *largest* eigenvalues of $I - L_{\text{sym}} = D^{-1/2}WD^{-1/2}$ and their eigenvectors. In fact, since the eigenvalues of L_{sym} are in the range $[0, 2]$, the eigenvalues of $2I - L_{\text{sym}} = I + D^{-1/2}WD^{-1/2}$ are also in the range $[0, 2]$ (that is, $I + D^{-1/2}WD^{-1/2}$ is positive semidefinite).

Let us now show how our original formulation (PNC1) can be converted to a more convenient form, by chasing the denominators in the Rayleigh ratios, and by expressing the objective function in terms of the *trace* of a certain matrix.

For any $N \times N$ matrix A, because

$$\begin{aligned} X^\top AX &= \begin{bmatrix} (X^1)^\top \\ \vdots \\ (X^K)^\top \end{bmatrix} A[X^1 \cdots X^K] \\ &= \begin{pmatrix} (X^1)^\top AX^1 & (X^1)^\top AX^2 & \cdots & (X^1)^\top AX^K \\ (X^2)^\top AX^1 & (X^2)^\top AX^2 & \cdots & (X^2)^\top AX^K \\ \vdots & \vdots & \ddots & \vdots \\ (X^K)^\top AX^1 & (X^K)^\top AX^2 & \cdots & (X^K)^\top AX^K \end{pmatrix}, \end{aligned}$$

we have

$$\operatorname{tr}(X^\top AX) = \sum_{j=1}^{K} (X^j)^\top AX^j,$$

and the conditions

$$(X^i)^\top AX^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j,$$

are equivalent to

$$X^\top AX = \operatorname{diag}((X^1)^\top AX^1, \ldots, (X^K)^\top AX^K).$$

As a consequence, if we assume that

$$(X^1)^\top AX^1 = \cdots = (X^K)^\top AX^K = \alpha^2,$$

then we have

$$X^\top AX = \alpha^2 I,$$

and if R is any orthogonal $K \times K$ matrix, then by multiplying on the left by $R^\top$ and on the right by R, we get

$$R^\top X^\top AXR = R^\top \alpha^2 IR = \alpha^2 R^\top R = \alpha^2 I.$$

Therefore, if

$$X^\top AX = \alpha^2 I,$$

then

$$(XR)^\top A(XR) = \alpha^2 I,$$

for any orthogonal $K \times K$ matrix R. Furthermore, because $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ for all matrices A, B, we have

$$\mathrm{tr}(R^\top X^\top A X R) = \mathrm{tr}(X^\top A X).$$

Since the Rayleigh ratios

$$\frac{(X^j)^\top L X^j}{(X^j)^\top D X^j}$$

are invariant under rescaling by a nonzero number, by replacing X^j by $((X^j)^\top D X^j)^{-1/2} X^j$, the denominators become 1, and we have

$$\begin{aligned}
\mu(X) = \mu(X^1, \ldots, X^K) &= \sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j} \\
&= \mu(((X^1)^\top D X^1)^{-1/2} X^1, \ldots, ((X^K)^\top D X^K)^{-1/2} X^K) \\
&= \sum_{j=1}^{K} ((X^j)^\top D X^j)^{-1/2} (X^j)^\top L \, ((X^j)^\top D X^j)^{-1/2} X^j \\
&= \mathrm{tr}(\Lambda^{-1/2} X^\top L X \Lambda^{-1/2}) \\
&= \mathrm{tr}(\Lambda^{-1} X^\top L X),
\end{aligned}$$

where

$$\Lambda = \mathrm{diag}((X^1)^\top D X^1, \ldots, (X^K)^\top D X^K).$$

If $(X^1)^\top D X^1 = \cdots = (X^K)^\top D X^K = \alpha^2$, then $\Lambda = \alpha^2 I_K$, so

$$\mu(X) = \mathrm{tr}(\Lambda^{-1} X^\top L X) = \frac{1}{\alpha^2} \mathrm{tr}(X^\top L X),$$

and for any orthogonal $K \times K$ matrix R,

$$\mu(RX) = \frac{1}{\alpha^2} \mathrm{tr}(R^\top X^\top L X R) = \frac{1}{\alpha^2} \mathrm{tr}(X^\top L X),$$

and thus,

$$\mu(X) = \mu(XR).$$

The condition

$$X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}$$

is also invariant if we replace X by XR, where R is any invertible matrix, because

$$\begin{aligned}
XR((XR)^\top (XR))^{-1} (XR)^\top \mathbf{1} &= XR(R^\top X^\top X R)^{-1} R^\top X^\top \mathbf{1} \\
&= XRR^{-1}(X^\top X)^{-1}(R^\top)^{-1} R^\top X^\top \mathbf{1} \\
&= X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}.
\end{aligned}$$

In summary we proved the following proposition:

Proposition 4.1. *For any orthogonal $K \times K$ matrix R, any symmetric $N \times N$ matrix A, and any $N \times K$ matrix $X = [X^1 \cdots X^K]$, the following properties hold:*

(1) $\mu(X) = \mathrm{tr}(\Lambda^{-1} X^\top L X)$, *where*

$$\Lambda = \mathrm{diag}((X^1)^\top D X^1, \ldots, (X^K)^\top D X^K).$$

(2) If $(X^1)^\top D X^1 = \cdots = (X^K)^\top D X^K = \alpha^2$, *then*

$$\mu(X) = \mu(XR) = \frac{1}{\alpha^2}\mathrm{tr}(X^\top L X).$$

(3) The condition $X^\top A X = \alpha^2 I$ *is preserved if* X *is replaced by* XR.

(4) The condition $X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}$ *is preserved if* X *is replaced by* XR.

Now, by Proposition 4.1(1) and the fact that the conditions in PNC1 are scale-invariant, we are led to the following formulation of our problem:

$$\begin{array}{lll}
\text{minimize} & \mathrm{tr}(X^\top L X) & \\
\text{subject to} & (X^i)^\top D X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, & \\
& (X^j)^\top D X^j = 1, \quad 1 \leq j \leq K, & \\
& X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}, & X \in \mathcal{X}.
\end{array}$$

Conditions on lines 2 and 3 can be combined in the equation

$$X^\top D X = I,$$

and, we obtain the following formulation of our minimization problem:

K-way Clustering of a graph using Normalized Cut, Version 2: Problem PNC2

$$\begin{array}{lll}
\text{minimize} & \mathrm{tr}(X^\top L X) & \\
\text{subject to} & X^\top D X = I, & \\
& X(X^\top X)^{-1} X^\top \mathbf{1} = \mathbf{1}, & X \in \mathcal{X}.
\end{array}$$

Because problem PNC2 requires the constraint $X^\top D X = I$ to be satisfied, it does not have the same set of solutions as problem PNC1. Nevertheless, problem PNC2 is equivalent to problem PNC1, in the sense that for every minimal solution $(X^1, \ldots, X^K)$ of PNC1, $(((X^1)^\top D X^1)^{-1/2} X^1, \ldots, ((X^K)^\top D X^K)^{-1/2} X^K)$ is a minimal solution of PNC2 (with the same minimum for the objective functions), and that for every minimal solution $(Z^1, \ldots, Z^k)$

of PNC2, $(\lambda_1 Z^1, \ldots, \lambda_K Z^K)$ is a minimal solution of PNC1, for all $\lambda_i \neq 0$, $i = 1, \ldots, K$ (with the same minimum for the objective functions). In other words, problems PNC1 and PNC2 have the same set of minimal solutions as K-tuples of points $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K))$ in $\mathbb{RP}^{N-1}$ determined by their homogeneous coordinates $X^1, \ldots, X^K$.

Formulation PNC2 reveals that finding a minimum normalized cut has a geometric interpretation in terms of the graph drawings discussed in Section 3.1. Indeed, PNC2 has the following equivalent formulation: Find a minimal energy graph drawing X in $\mathbb{R}^K$ of the weighted graph $G = (V, W)$ such that:

1. The matrix X is orthogonal with respect to the inner product $\langle -, - \rangle_D$ in $\mathbb{R}^N$ induced by D, with
$$\langle x, y \rangle_D = x^\top D y, \quad x, y \in \mathbb{R}^N.$$

2. The rows of X are nonzero; this means that no vertex $v_i \in V$ is assigned to the origin of $\mathbb{R}^K$ (the zero vector 0_K).

3. Every vertex v_i is assigned a point of the form $(0, \ldots, 0, a_j, 0, \ldots, 0)$ on some axis (in $\mathbb{R}^K$).

4. Every axis in $\mathbb{R}^K$ is assigned at least some vertex.

Condition 1 can be reduced to the standard condition for graph drawings ($R^\top R = I$) by making the change of variable $Y = D^{1/2} X$ or equivalently $X = D^{-1/2} Y$. Indeed,

$$\mathrm{tr}(X^\top L X) = \mathrm{tr}(Y^\top D^{-1/2} L D^{-1/2} Y),$$

so we use the normalized Laplacian $L_{\mathrm{sym}} = D^{-1/2} L D^{-1/2}$ instead of L,

$$X^\top D X = Y^\top Y = I,$$

and conditions (2), (3), (4) are preserved under the change of variable $Y = D^{1/2} X$, since $D^{1/2}$ is invertible. However, conditions (2), (3), (4) are "hard" constraints, especially condition (3). In fact, condition (3) implies that the columns of X are orthogonal with respect to both the Euclidean inner product and the inner product $\langle -, - \rangle_D$, so condition (1) is redundant, except for the fact that it prescribes the norm of the columns, but this is not essential due to the projective nature of the solutions.

The main problem in finding a good relaxation of problem PNC2 is that it is very difficult to enforce the condition $X \in \mathcal{X}$. Also, the solutions X are not preserved under arbitrary rotations, but only by very special rotations which leave $\mathcal{X}$ invariant (they exchange the axes).

The first natural relaxation of problem PNC2 is to drop the condition that $X \in \mathcal{X}$, and we obtain the

Problem $(*_2)$

$$\begin{array}{ll} \text{minimize} & \operatorname{tr}(X^\top LX) \\ \text{subject to} & X^\top DX = I, \\ & X(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1}. \end{array}$$

Actually, since the discrete solutions $X \in \mathcal{X}$ that we are ultimately seeking are solutions of problem PNC1, the preferred relaxation is the one obtained from problem PNC1 by dropping the condition $X \in \mathcal{X}$, and simply requiring that $X^j \neq 0$, for $j = 1, \ldots, K$:

Problem $(*_1)$

$$\begin{array}{lll} \text{minimize} & \displaystyle\sum_{j=1}^{K} \frac{(X^j)^\top LX^j}{(X^j)^\top DX^j} & \\ \text{subject to} & (X^i)^\top DX^j = 0, \quad X^j \neq 0 & 1 \leq i, j \leq K,\ i \neq j, \\ & X(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1}. & \end{array}$$

Now that we dropped the condition $X \in \mathcal{X}$, it is not clear that $X^\top X$ is invertible in $(*_1)$ and $(*_2)$. However, since the columns of X are nonzero and D-orthogonal, they must be linearly independent, so X has rank K and and $X^\top X$ is invertible.

As we explained before, every solution $Z = [Z^1, \ldots, Z^K]$ of problem $(*_1)$ yields a solution of problem $(*_2)$ by normalizing each Z^j by $((Z^j)^\top DZ^j)^{1/2}$, and conversely for every solution $Z = [Z^1, \ldots, Z^K]$ of problem $(*_2)$, the K-tuple $[\lambda_1 Z^1, \ldots, \lambda_K Z^K]$ is a solution of problem $(*_1)$, where $\lambda_j \neq 0$ for $j = 1, \ldots, K$. Furthermore, by Proposition 4.1, for every orthogonal matrix $R \in \mathbf{O}(K)$ and for every solution X of $(*_2)$, the matrix XR is also a solution of $(*_2)$. Since Proposition 4.1(2) requires that all $(X^j)^\top DX^j$ have the same value in order to have $\mu(X) = \mu(XR)$, in general, if X is a solution of $(*_1)$, the matrix XR is not necessarily a solution of $(*_1)$. However, every solution X of $(*_2)$ is also a solution of $(*_1)$, for every $R \in \mathbf{O}(K)$, XR is a solution of both $(*_2)$ and $(*_1)$, and since $(*_1)$ is scale-invariant, for every diagonal invertible matrix Λ, the matrix $XR\Lambda$ is a solution of $(*_1)$.

In summary, every solution Z of problem $(*_2)$ yields a *family of solutions* of problem $(*_1)$; namely, all matrices of the form $ZR\Lambda$, where $R \in \mathbf{O}(K)$ and Λ is a diagonal invertible matrix. We will take advantage of this fact in looking for a discrete solution X "close" to a solution Z of the relaxed problem $(*_2)$.

Observe that a matrix is of the form $R\Lambda$ with $R \in \mathbf{O}(K)$ and Λ a diagonal invertible matrix iff its columns are nonzero and pairwise orthogonal. First, we have

$$(R\Lambda)^\top R\Lambda = \Lambda^\top R^\top R\Lambda = \Lambda^2,$$

which implies that the columns of $R\Lambda$ are nonzero and pairwise orthogonal. Conversely, if the columns of A are nonzero and pairwise orthogonal, then

$$A^\top A = \Lambda^2$$

for some invertible diagonal matrix Λ, and then $A = R\Lambda$, where $R = A\Lambda^{-1}$ is orthogonal.

As a consequence of the invariance of solutions of $(*_2)$ under multiplication on the right by matrices in $\mathbf{O}(K)$, as explained below, we can view the solutions of problem $(*_2)$ as elements of the *Grassmannian* $G(K, N)$.

Recall that the *Stiefel manifold* $St(k, n)$ consists of the set of orthogonal k-frames in $\mathbb{R}^n$, that is, the k-tuples of orthonormal vectors $(u_1, \ldots, u_k)$ with $u_i \in \mathbb{R}^n$. For $k = n$, the manifold $St(n, n)$ is identical to the orthogonal group $\mathbf{O}(n)$. For $1 \leq n \leq n-1$, the group $\mathbf{SO}(n)$ acts transitively on $St(k, n)$, and $St(k, n)$ is isomorphic to the coset manifold $\mathbf{SO}(n)/\mathbf{SO}(n-k)$. The *Grassmann manifold* $G(k, n)$ consists of all (linear) k-dimensional subspaces of $\mathbb{R}^n$. Again, the group $\mathbf{SO}(n)$ acts transitively on $G(k, n)$, and $G(k, n)$ is isomorphic to the coset manifold $\mathbf{SO}(n)/S(\mathbf{O}(k) \times \mathbf{O}(n-k))$. The group $\mathbf{O}(k)$ acts on the right on the Stiefel manifold $St(k, n)$ (by multiplication), and the orbit manifold $St(k, n)/\mathbf{O}(k)$ is isomorphic to the Grassmann manifold $G(k, n)$. Furthermore, both $St(k, n)$ and $G(k, n)$ are *naturally reductive homogeneous manifolds* (for the Stiefel manifold, when $n \geq 3$), and $G(k, n)$ is even a *symmetric space* (see O'Neill [18]). The upshot of all this is that to a large extent, the differential geometry of these manifolds is completely determined by some subspace $\mathfrak{m}$ of the Lie algebra $\mathfrak{so}(n)$, such that we have a direct sum

$$\mathfrak{so}(n) = \mathfrak{m} \oplus \mathfrak{h},$$

where $\mathfrak{h} = \mathfrak{so}(n-k)$ in the case of the Stiefel manifold, and $\mathfrak{h} = \mathfrak{so}(k) \times \mathfrak{so}(n-k)$ in the case of the Grassmannian manifold (some additional condition on $\mathfrak{m}$ is required). In particular, the geodesics in both manifolds can be determined quite explicitly, and thus we obtain closed form formulae for distances, *etc.*

The Stiefel manifold $St(k, n)$ can be viewed as the set of all $n \times k$ matrices X such that

$$X^\top X = I_k.$$

In our situation, we are considering $N \times K$ matrices X such that

$$X^\top D X = I.$$

This is not quite the Stiefel manifold, but if we write $Y = D^{1/2}X$, then we have

$$Y^\top Y = I,$$

so the space of matrices X satisfying the condition $X^\top D X = I$ is the image $\mathcal{D}(St(K, N))$ of the Stiefel manifold $St(K, N)$ under the linear map $\mathcal{D}$ given by

$$\mathcal{D}(X) = D^{1/2}X.$$

Now, the right action of $\mathbf{O}(K)$ on $\mathcal{D}(St(K, N))$ yields a coset manifold $\mathcal{D}(St(K, N))/\mathbf{O}(K)$ which is obviously isomorphic to the Grassmann manidold $G(K, N)$.

Therefore, *the solutions of problem* $(*_2)$ *can be viewed as elements of the Grassmannian* $G(K, N)$. We can take advantage of this fact to find a discrete solution of our original optimization problem PNC2 approximated by a continuous solution of $(*_2)$.

Recall that if $X^\top X$ is invertible (which is the case), condition $X(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1}$ is equivalent to $XX^+\mathbf{1} = \mathbf{1}$, which is also equivalent to the fact that $\mathbf{1}$ is in the range of X. If we make the change of variable $Y = D^{1/2}X$ or equivalently $X = D^{-1/2}Y$, the condition that $\mathbf{1}$ is in the range of X becomes the condition that $D^{1/2}\mathbf{1}$ is in the range of Y, which is equivalent to

$$YY^+D^{1/2}\mathbf{1} = D^{1/2}\mathbf{1}.$$

However, since $Y^\top Y = I$, we have

$$Y^+ = Y^\top,$$

so we get the equivalent problem

Problem $(**_2)$

$$\begin{array}{ll} \text{minimize} & \operatorname{tr}(Y^\top D^{-1/2}LD^{-1/2}Y) \\ \text{subject to} & Y^\top Y = I, \\ & YY^\top D^{1/2}\mathbf{1} = D^{1/2}\mathbf{1}. \end{array}$$

This time, the matrices Y satisfying condition $Y^\top Y = I$ do belong to the Stiefel manifold $St(K, N)$, and again, *we view the solutions of problem* $(**_2)$ *as elements of the Grassmannian* $G(K, N)$. We pass from a solution Y of problem $(**_2)$ in $G(K, N)$ to a solution Z of of problem $(*_2)$ in $G(K, N)$ by the linear map $\mathcal{D}^{-1}$; namely, $Z = \mathcal{D}^{-1}(Y) = D^{-1/2}Y$.

It is not a priori obvious that the minimum of $\operatorname{tr}(Y^\top L_{\text{sym}}Y)$ over all $N \times K$ matrices Y satisfying $Y^\top Y = I$ is equal to the sum $\nu_1 + \cdots + \nu_K$ of the first K eigenvalues of $L_{\text{sym}} = D^{-1/2}LD^{-1/2}$. Fortunately, the Poincaré separation theorem (Proposition A.3) guarantees that the sum of the K smallest eigenvalues of L_{sym} is a lower bound for $\operatorname{tr}(Y^\top L_{\text{sym}}Y)$. Furthermore, if we temporarily ignore the second constraint, the minimum of problem $(**_2)$ is achieved by any K unit eigenvectors $(u_1, \ldots, u_K)$ associated with the smallest eigenvalues

$$0 = \nu_1 \leq \nu_2 \leq \ldots \leq \nu_K$$

of L_{sym}.[1] We may assume that $\nu_2 > 0$, namely that the underlying graph is connected (otherwise, we work with each connected component), in which case $Y^1 = D^{1/2}\mathbf{1}/\left\|D^{1/2}\mathbf{1}\right\|_2$, because $\mathbf{1}$ is in the nullspace of L. Since $Y^1 = D^{1/2}\mathbf{1}/\left\|D^{1/2}\mathbf{1}\right\|_2$, the vector $D^{1/2}\mathbf{1}$ is in the range of Y, so the condition

$$YY^\top D^{1/2}\mathbf{1} = D^{1/2}\mathbf{1}$$

[1] Other authors seem to accept this fact as obvious. This is not quite so, and Godsil and Royle [10] provide a rigorous proof using Proposition A.3.

is also satisfied. Then, $Z = D^{-1/2}Y$ with $Y = [u_1 \ \ldots \ u_K]$ yields a minimum of our relaxed problem $(*_2)$ (the second constraint is satisfied because $\mathbf{1}$ is in the range of Z).

By Proposition 2.6, the vectors Z^j are eigenvectors of L_{rw} associated with the eigenvalues $0 = \nu_1 \leq \nu_2 \leq \ldots \leq \nu_K$. Recall that $\mathbf{1}$ is an eigenvector for the eigenvalue $\nu_1 = 0$, and $Z^1 = \mathbf{1}/\left\|D^{1/2}\mathbf{1}\right\|_2$. Because, $(Y^i)^\top Y^j = 0$ whenever $i \neq j$, we have

$$(Z^i)^\top D Z^j = 0, \quad \text{whenever } i \neq j.$$

This implies that $Z^2, \ldots, Z^K$ are all orthogonal to $D\mathbf{1}$, and thus, that each Z^j has both some positive and some negative coordinate, for $j = 2, \ldots, K$.

The conditions $(Z^i)^\top D Z^j = 0$ do not necessarily imply that Z^i and Z^j are orthogonal (w.r.t. the Euclidean inner product), but we can obtain a solution of Problems $(*_2)$ and $(*_1)$ achieving the same minimum for which distinct columns Z^i and Z^j are simultaneously orthogonal and D-orthogonal, by multiplying Z by some $K \times K$ orthogonal matrix R on the right. Indeed, if Z is a solution of $(*_2)$ obtained as above, the $K \times K$ symmetric matrix $Z^\top Z$ can be diagonalized by some orthogonal $K \times K$ matrix R as

$$Z^\top Z = R \Sigma R^\top,$$

where Σ is a diagonal matrix, and thus,

$$R^\top Z^\top Z R = (ZR)^\top ZR = \Sigma,$$

which shows that the columns of ZR are orthogonal. By Proposition 4.1, ZR also satisfies the constraints of $(*_2)$ and $(*_1)$, and $\mathrm{tr}((ZR)^\top L(ZR)) = \mathrm{tr}(Z^\top LZ)$.

Remark: Since Y has linearly independent columns (in fact, orthogonal) and since $Z = D^{-1/2}Y$, the matrix Z also has linearly independent columns, so $Z^\top Z$ is positive definite and the entries in Σ are all positive. Also, instead of computing $Z^\top Z$ explicitly and diagonalizing it, the matrix R can be found by computing an SVD of Z.

In summary, we should look for a solution Z of $(*_2)$ that corresponds to an element of the Grassmannian $G(K, N)$, and hope that for some suitable orthogonal matrix R and some diagonal invertible matrix Λ, the vectors in $XR\Lambda$ are close to a true solution of the original problem.

4.4 K-Way Clustering; Using The Dependencies Among $X^1, \ldots, X^K$

At this stage, it is interesting to reconsider the case $K = 2$ in the light of what we just did when $K \geq 3$. When $K = 2$, X^1 and X^2 are not independent, and it is convenient to assume that the nonzero entries in X^1 and X^2 are both equal to some positive real $c \in \mathbb{R}$, so that

$$X^1 + X^2 = c\mathbf{1}.$$

To avoid subscripts, write $(A, \overline{A})$ for the partition of V that we are seeking, and as before let $d = \mathbf{1}^\top D\mathbf{1}$ and $\alpha = \mathrm{vol}(A)$. We know from Section 4.2 that

$$(X^1)^\top DX^1 = \alpha c^2$$
$$(X^2)^\top DX^2 = (d-\alpha)c^2,$$

so we normalize X^1 and X^2 so that $(X^1)^\top DX^1 = (X^2)^\top DX^2 = c^2$, and we consider

$$X = \begin{bmatrix} \dfrac{X^1}{\sqrt{\alpha}} & \dfrac{X^2}{\sqrt{d-\alpha}} \end{bmatrix}.$$

Now, we claim that there is an orthogonal matrix R so that if X as above is a solution to our discrete problem, then XR contains a multiple of $\mathbf{1}$ as a first column. A similar observation is made in Yu [23] and Yu and Shi [24] (but beware that in these works $\alpha = \mathrm{vol}(A)/\sqrt{d}$). In fact,

$$R = \frac{1}{\sqrt{d}} \begin{pmatrix} \sqrt{\alpha} & \sqrt{d-\alpha} \\ \sqrt{d-\alpha} & -\sqrt{\alpha} \end{pmatrix}.$$

Indeed, we have

$$\begin{aligned} XR &= \begin{bmatrix} \dfrac{X^1}{\sqrt{\alpha}} & \dfrac{c\mathbf{1} - X^1}{\sqrt{d-\alpha}} \end{bmatrix} R \\ &= \begin{bmatrix} \dfrac{X^1}{\sqrt{\alpha}} & \dfrac{c\mathbf{1} - X^1}{\sqrt{d-\alpha}} \end{bmatrix} \frac{1}{\sqrt{d}} \begin{pmatrix} \sqrt{\alpha} & \sqrt{d-\alpha} \\ \sqrt{d-\alpha} & -\sqrt{\alpha} \end{pmatrix} \\ &= \frac{1}{\sqrt{d}} \left[c\mathbf{1} \;\; \sqrt{\frac{d-\alpha}{\alpha}}\, X^1 - \sqrt{\frac{\alpha}{d-\alpha}}\, (c\mathbf{1} - X^1) \right]. \end{aligned}$$

If we let

$$a = c\sqrt{\frac{d-\alpha}{\alpha}}, \quad b = -c\sqrt{\frac{\alpha}{d-\alpha}},$$

then we check that

$$\alpha a + b(d-\alpha) = 0,$$

which shows that the vector

$$Z = \sqrt{\frac{d-\alpha}{d\alpha}}\, X^1 - \sqrt{\frac{\alpha}{d(d-\alpha)}}\, (c\mathbf{1} - X^1)$$

is a potential solution of our discrete problem in the sense of Section 4.2. Furthermore, because $L\mathbf{1} = 0$,

$$\mathrm{tr}(X^\top LX) = \mathrm{tr}((XR)^\top L(XR)) = Z^\top LZ,$$

the vector Z is indeed a solution of our discrete problem. Thus, we reconfirm the fact that the second eigenvector of $L_{\mathrm{rw}} = D^{-1}L$ is indeed a continuous approximation to the clustering problem when $K = 2$. This can be generalized for any $K \geq 2$.

Again, we may assume that the nonzero entries in $X^1, \ldots, X^K$ are some positive real $c \in \mathbb{R}$, so that

$$X^1 + \cdots + X^K = c\mathbf{1},$$

and if $(A_1, \ldots, A_K)$ is the partition of V that we are seeking, write $\alpha_j = \mathrm{vol}(A_j)$. We have $\alpha_1 + \cdots + \alpha_K = d = \mathbf{1}^\top D\mathbf{1}$. Since

$$(X^j)^\top D X^j = \alpha_j c^2,$$

we normalize the X^j so that $(X^j)^\top D X^j = \cdots = (X^K)^\top D X^K = c^2$, and we consider

$$X = \begin{bmatrix} \dfrac{X^1}{\sqrt{\alpha_1}} & \dfrac{X^2}{\sqrt{\alpha_2}} & \cdots & \dfrac{X^K}{\sqrt{\alpha_K}} \end{bmatrix}.$$

Then, we have the following result.

Proposition 4.2. *If* $X = \begin{bmatrix} \frac{X^1}{\sqrt{\alpha_1}} & \frac{X^2}{\sqrt{\alpha_2}} & \cdots & \frac{X^K}{\sqrt{\alpha_K}} \end{bmatrix}$ *is a solution of our discrete problem, then there is an orthogonal matrix* R *such that its first column* R^1 *is*

$$R^1 = \frac{1}{\sqrt{d}} \begin{pmatrix} \sqrt{\alpha_1} \\ \sqrt{\alpha_2} \\ \vdots \\ \sqrt{\alpha_K} \end{pmatrix}$$

and

$$XR = \begin{bmatrix} \dfrac{c}{\sqrt{d}}\mathbf{1} & Z^2 & \cdots & Z^K \end{bmatrix}.$$

Furthermore,

$$(XR)^\top D(XR) = c^2 I$$

and

$$\mathrm{tr}((XR)^\top L(XR)) = \mathrm{tr}(Z^\top L Z),$$

with $Z = [Z^2 \cdots Z^K]$.

Proof. Apply Gram–Schmidt to $(R^1, e_2, \ldots, e_K)$ (where $(e_1, \ldots, e_K)$ is the canonical basis of $\mathbb{R}^K$) to form an orthonormal basis. The rest follows from Proposition 4.1. □

Proposition 4.2 suggests that if $Z = [\mathbf{1}\ Z^2 \cdots Z^K]$ is a solution of the relaxed problem $(*_2)$, then there should be an orthogonal matrix R such that $ZR^\top$ is an approximation of a solution of the discrete problem PNC1.

4.5 Finding a Discrete Solution Close to a Continuous Approximation

The next step is to find an exact solution $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)) \in \mathbb{P}(\mathcal{K})$ which is the closest (in a suitable sense) to our approximate solution $(Z^1, \ldots, Z^K) \in G(K, N)$. The set $\mathcal{K}$ is closed under very special orthogonal transformations in $\mathbf{O}(K)$, so we can't view $\mathcal{K}$ as a subset of the Grassmannian $G(K, N)$. However, we can think of $\mathcal{K}$ as a subset of $G(K, N)$ by considering the subspace spanned by $(X^1, \ldots, X^K)$ for every $[X^1 \ \cdots X^K\,] \in \mathcal{K}$.

Recall from Section 4.3 that every solution Z of problem $(*_2)$ yields a *family of solutions* of problem $(*_1)$; namely, all matrices of the form ZQ, where Q is a $K \times K$ matrix with nonzero and pairwise orthogonal columns. Since the solutions ZQ of $(*_1)$ are all equivalent (they yield the same minimum for the normalized cut), it makes sense to look for a discrete solution X closest to one of these ZQ. Then, we have two choices of distances.

1. We view $\mathcal{K}$ as a subset of $(\mathbb{RP}^{N-1})^K$. Because $\mathcal{K}$ is closed under the antipodal map, as explained in Appendix B, for every j $(1 \leq j \leq K)$, minimizing the distance $d(\mathbb{P}(X^j), \mathbb{P}(Z^j))$ on $\mathbb{RP}^{N-1}$ is equivalent to minimizing $\|X^j - Z^j\|_2$, where X^j and Z^j are representatives of $\mathbb{P}(X^j)$ and $\mathbb{P}(Z^j)$ on the unit sphere (if we use the Riemannian metric on $\mathbb{RP}^{N-1}$ induced by the Euclidean metric on $\mathbb{R}^N$). Then, if we use the product distance on $(\mathbb{RP}^{N-1})^K$ given by

$$d\big((\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)), (\mathbb{P}(Z^1), \ldots, \mathbb{P}(Z^K))\big) = \sum_{j=1}^{K} d(\mathbb{P}(X^j), \mathbb{P}(Z^j)),$$

minimizing the distance $d\big((\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K)), (\mathbb{P}(Z^1), \ldots, \mathbb{P}(Z^K))\big)$ in $(\mathbb{RP}^{N-1})^K$ is equivalent to minimizing

$$\sum_{j=1}^{K} \left\|X^j - Z^j\right\|_2, \quad \text{subject to} \quad \left\|X^j\right\|_2 = \left\|Z^j\right\|_2 \ (j = 1, \ldots, K).$$

We are not aware of any optimization method to solve the above problem, which seems difficult to tackle due to constraints $\|X^j\|_2 = \|Z^j\|_2$ $(j = 1, \ldots, K)$. Therefore, we drop these constraints and attempt to minimize

$$\|X - Z\|_F^2 = \sum_{j=1}^{K} \left\|X^j - Z^j\right\|_2^2,$$

the Frobenius norm of $X - Z$. This is implicitly the choice made by Yu.

2. We view $\mathcal{K}$ as a subset of the Grassmannian $G(K, N)$. In this case, we need to pick a metric on the Grassmannian, and we minimize the corresponding Riemannian distance $d(X, Z)$. A natural choice is the metric on $\mathfrak{so}(n)$ given by

$$\langle X, Y \rangle = \operatorname{tr}(X^\top Y).$$

This choice remains to be explored.

Inspired by Yu [23] and the previous discussion, given a solution Z of problem $(*_2)$, we look for pairs (X, Q) with $X \in \mathcal{X}$ and where Q is a $K \times K$ matrix with nonzero and pairwise orthogonal columns, with $\|X\|_F = \|Z\|_F$, that minimize

$$\varphi(X, Q) = \|X - ZQ\|_F .$$

Here, $\|A\|_F$ is the Frobenius norm of A, with $\|A\|_F^2 = \mathrm{tr}(A^\top A)$. Yu [23] and Yu and Shi [24] consider the special case where $Q \in \mathbf{O}(K)$. We consider the more general case where $Q = R\Lambda$, with $R \in \mathbf{O}(K)$ and Λ is a diagonal invertible matrix.

The key to minimizing $\|X - ZQ\|_F$ rests on the following computation:

$$\begin{aligned}
\|X - ZQ\|_F^2 &= \mathrm{tr}((X - ZQ)^\top (X - ZQ)) \\
&= \mathrm{tr}((X^\top - Q^\top Z^\top)(X - ZQ)) \\
&= \mathrm{tr}(X^\top X - X^\top ZQ - Q^\top Z^\top X + Q^\top Z^\top ZQ) \\
&= \mathrm{tr}(X^\top X) - \mathrm{tr}(X^\top ZQ) - \mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Q^\top Z^\top ZQ) \\
&= \mathrm{tr}(X^\top X) - \mathrm{tr}((Q^\top Z^\top X)^\top) - \mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Z^\top ZQQ^\top) \\
&= \|X\|_F^2 - 2\mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Z^\top ZQQ^\top).
\end{aligned}$$

Therefore, since $\|X\|_F = \|Z\|_F$ is fixed, minimizing $\|X - ZQ\|_F^2$ is equivalent to minimizing $-2\mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Z^\top ZQQ^\top)$.

This is a hard problem because it is a nonlinear optimization problem involving two matrix unknowns X and Q. To simplify the problem, we proceed by alternating steps during which we minimize $\varphi(X, Q) = \|X - ZQ\|_F$ with respect to X holding Q fixed, and steps during which we minimize $\varphi(X, Q) = \|X - ZQ\|_F$ with respect to Q holding X fixed.

This second step in which X is held fixed has been studied, but it is still a hard problem for which no closed–form solution is known. Consequently, we further simplify the problem. Since Q is of the form $Q = R\Lambda$ where $R \in \mathbf{O}(K)$ and Λ is a diagonal invertible matrix, we minimize $\|X - ZR\Lambda\|_F$ in two stages.

1. We set $\Lambda = I$ and find $R \in \mathbf{O}(K)$ that minimizes $\|X - ZR\|_F$.

2. Given X, Z, and R, find a diagonal invertible matrix Λ that minimizes $\|X - ZR\Lambda\|_F$.

The matrix $R\Lambda$ is not a minimizer of $\|X - ZR\Lambda\|_F$ in general, but it is an improvement on R alone, and both stages can be solved quite easily.

In stage 1, the matrix $Q = R$ is orthogonal, so $QQ^\top = I$, and since Z and X are given, the problem reduces to minimizing $-2\mathrm{tr}(Q^\top Z^\top X)$; that is, maximizing $\mathrm{tr}(Q^\top Z^\top X)$. To solve this problem, we need the following proposition.

Proposition 4.3. *For any $n \times n$ matrix A and any orthogonal matrix Q, we have*

$$\max\{\mathrm{tr}(QA) \mid Q \in \mathbf{O}(n)\} = \sigma_1 + \cdots + \sigma_n,$$

where $\sigma_1 \geq \cdots \geq \sigma_n$ are the singular values of A. Furthermore, this maximum is achieved by $Q = VU^\top$, where $A = U\Sigma V^\top$ is any SVD for A.

Proof. Let $A = U\Sigma V^\top$ be any SVD for A. Then we have

$$\begin{aligned}\mathrm{tr}(QA) &= \mathrm{tr}(QU\Sigma V^\top)\\ &= \mathrm{tr}(V^\top QU\Sigma).\end{aligned}$$

The matrix $Z = V^\top QU$ is an orthogonal matrix so $|z_{ij}| \leq 1$ for $1 \leq i, j \leq n$, and Σ is a diagonal matrix, so we have

$$\mathrm{tr}(Z\Sigma) = z_{11}\sigma_1 + \cdots + z_{nn}\sigma_n \leq \sigma_1 + \cdots + \sigma_n,$$

which proves the first statement of the proposition. For $Q = VU^\top$, we get

$$\begin{aligned}\mathrm{tr}(QA) &= \mathrm{tr}(QU\Sigma V^\top)\\ &= \mathrm{tr}(VU^\top U\Sigma V^\top)\\ &= \mathrm{tr}(V\Sigma V^\top) = \sigma_1 + \cdots + \sigma_n,\end{aligned}$$

which proves the second part of the proposition. □

As a corollary of Proposition 4.3 (with $A = Z^\top X$ and $Q = R^\top$), we get the following result (see Golub and Van Loan [11], Section 12.4.1):

Proposition 4.4. *For any two fixed $N \times K$ matrices X and Z, the minimum of the set*

$$\{\|X - ZR\|_F \mid R \in \mathbf{O}(K)\}$$

is achieved by $R = UV^\top$, for any SVD decomposition $U\Sigma V^\top = Z^\top X$ of $Z^\top X$.

The following proposition takes care of stage 2.

Proposition 4.5. *For any two fixed $N \times K$ matrices X and Z, where Z has no zero column, there is a unique diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_K)$ minimizing $\|X - Z\Lambda\|_F$ given by*

$$\lambda_j = \frac{(Z^\top X)_{jj}}{\|Z^j\|_2^2} \quad j = 1, \ldots, K.$$

Proof. Since Λ is a diagonal matrix, we have

$$\begin{aligned}\|X - Z\Lambda\|^2 &= \|X\|_2^2 - 2\mathrm{tr}(\Lambda^\top Z^\top X) + \mathrm{tr}(Z^\top Z\Lambda\Lambda^\top)\\ &= \|X\|_2^2 - 2\mathrm{tr}(Z^\top X\Lambda) + \mathrm{tr}(Z^\top Z\Lambda^2)\\ &= \|X\|_2^2 - 2\sum_{j=1}^{K}(Z^\top X)_{jj}\lambda_j + \sum_{j=1}^{K}\left\|Z^j\right\|_2^2\lambda_j^2.\end{aligned}$$

The above functional has a critical point obtained by setting the partial derivatives with respect to the λ_j to 0, which gives

$$-2(Z^\top X)_{jj} + 2\left\|Z^j\right\|_2^2 \lambda_j = 0;$$

that is,

$$\lambda_j = \frac{(Z^\top X)_{jj}}{\|Z^j\|_2^2}.$$

Since the functional is a sum of quadratic functions and the coefficients $\|Z^j\|_2^2$ of the λ_j^2 are positive, this critical point is indeed a minimum. □

It should be noted that Proposition 4.5 does not guarantee that Λ is invertible. For example, for

$$X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & -1 \end{pmatrix},$$

we have

$$Z^\top X = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & 0 \end{pmatrix},$$

so $\lambda_2 = 0$. When Proposition 4.5 yields a singular matrix, we skip stage 2 (we set $\Lambda = I$).

We now deal with step 1, where $Q = R\Lambda$ is held fixed. For fixed Z and Q, we would like to find some $X \in \mathcal{K}$ with $\|X\|_F = \|Z\|_F$ so that $\|X - ZQ\|_F$ is minimal. Without loss of generality, we may assume that the entries $a_1, \ldots, a_K$ occurring in the matrix X are positive and all equal to some common value $a \neq 0$. Recall that a matrix $X \in \mathcal{X}$ has the property that every row contains exactly one nonzero entry, and that every column is nonzero.

To find $X \in \mathcal{K}$, first we find the shape $\widehat{X}$ of X, which is the matrix obtained from X by rescaling the columns of X so that $\widehat{X}$ has entries $+1, 0$. The problem is to decide for each row, which column contains the nonzero entry. After having found $\widehat{X}$, we rescale its columns so that $\|X\|_F = \|Z\|_F$.

Since

$$\|X - ZQ\|_F^2 = \|X\|_F^2 - 2\mathrm{tr}(Q^\top Z^\top X) + \mathrm{tr}(Z^\top ZQQ^\top),$$

minimizing $\|X - ZQ\|_F$ is equivalent to maximizing

$$\mathrm{tr}(Q^\top Z^\top X) = \mathrm{tr}((ZQ)^\top X) = \mathrm{tr}(X(ZQ)^\top),$$

and since the ith row of X contains a single nonzero entry a in column j_i ($1 \leq j_i \leq K$), if we write $Y = ZQ$, then

$$\mathrm{tr}(XY^\top) = a \sum_{i=1}^{N} y_{i\, j_i}. \qquad (*)$$

By $(*)$, since $a > 0$, the quantity $\mathrm{tr}(XY^\top)$ is maximized iff y_{ij_i} is maximized for $i = 1, \ldots, N$; this is achieved if for the ith row of X, we pick a column index ℓ such that $y_{i\ell}$ is maximum.

To find the shape $\widehat{X}$ of X, we first find a matrix $\overline{X}$ by chosing a single nonzero entry $\overline{x}_{ij} = 1$ on row i in such a way that y_{ij} is maximum according to the following method. If we let

$$\mu_i = \max_{1 \leq j \leq K} y_{ij}$$
$$J_i = \{j \in \{1, \ldots, K\} \mid y_{ij} = \mu_i\},$$

for $i = 1, \ldots, N$, then

$$\overline{x}_{ij} = \begin{cases} +1 & \text{for some chosen } j \in J_i, \\ 0 & \text{otherwise.} \end{cases}$$

Of course, a single column index is chosen for each row. In our implementation, we pick the smallest index in J_i.

Unfortunately, the matrix $\overline{X}$ may not be a correct solution, because the above prescription does not guarantee that every column of $\overline{X}$ is nonzero. When this happens, we reassign certain nonzero entries in columns having "many" nonzero entries to zero columns, so that we get a matrix in $\mathcal{K}$.

Suppose column j is zero. Then, we pick the leftmost index k of a column with a maximum number of 1, and if i the smallest index for which $\overline{X}_{ik} = 1$, then we set $\overline{X}_{ik} = 0$ and $\overline{X}_{ij} = 1$. We repeat this reallocation scheme until every column is nonzero.

We obtain a new matrix $\widehat{X}$ in $\mathcal{X}$, and finally we normalize $\widehat{X}$ to obtain X, so that $\|X\|_F = \|Z\|_F$.

A practical way to deal with zero columns in $\overline{X}$ is to simply decrease K. Clearly, further work is needed to justify the soundness of such a method.

The above method is essentially the method described in Yu [23] and Yu and Shi [24], except that in these works (in which X, Z and Y are denoted by $X^*, \widetilde{X}^*$, and $\widetilde{X}$, respectively) the entries in X belong to $\{0, 1\}$; as described above, for row i, the index ℓ corresponding to the entry $+1$ is given by

$$\arg \max_{1 \leq j \leq K} \widetilde{X}(i, j).$$

The fact that $\overline{X}$ may have zero columns is not addressed by Yu. Furthermore, it is important to make sure that X has the same norm as Z, but this normalization step is not performed in the above works. On the other hand, the rows of Z are normalized and the resulting matrix may no longer be a correct solution of the relaxed problem. In practice, it appears to be a good approximation of a discrete solution; see option (3) of the initialization methods for Z described below.

Any matrix obtained by flipping the signs of some of the columns of a solution ZR of problem $(*_2)$ is still a solution. Moreover, all entries in X are nonnegative. It follows that

a "good" solution ZQ_p (that is, close to a discrete solution) should have the property that the average of each of its column is nonnegative. We found that the following heuristic is quite helpful in finding a better discrete solution X. Given a solution ZR of problem $(*_2)$, we compute ZQ_p, defined such that if the average of column $(ZR)^j$ is negative, then $(ZQ_p)^j = -(ZR)^j$, else $(ZQ_p)^j = (ZR)^j$. It follows that the average of every column in ZQ_p is nonnegative. Then, we apply the above procedure to find discrete solutions X and X_p closest to ZR and ZQ_p respectively, and we pick the solution corresponding to $\min\{\|X - ZR\|_F, \|X_p - ZQ_p\|_F\}$. Flipping signs of columns of ZR correspond to a diagonal matrix R_p with entries ± 1, a very special kind of orthogonal matrix. In summary, the procedure for finding a discrete X close to a continuous ZR also updates R to $Q_p = RR_p$. This step appears to be very effective for finding a good initial X.

The method due to Yu and Shi (see Yu [23] and Yu and Shi [24]) to find $X \in \mathcal{K}$ and $Q = R\Lambda$ with $R \in \mathbf{O}(K)$ and Λ diagonal invertible that minimize $\varphi(X, Q) = \|X - ZQ\|_F$ is to alternate steps during which either Q is held fixed (step PODX) or X is held fixed (step PODR), except that Yu and Shi consider the special case where $\Lambda = I$.

(1) In step PODX, the next discrete solution X^* is obtained fom the previous pair (Q^*, Z) by computing $\overline{X}$ and then $X^* = \widehat{X}$ from $Y = ZQ^*$, as just explained above.

(2) In step PODR, the next matrix $Q^* = R\Lambda$ is obtained from the previous pair (X^*, Z) by first computing

$$R = UV^\top,$$

for any SVD decomposition $U\Sigma V^\top$ of $Z^\top X^*$, and then computing Λ from X^* and ZR using Proposition 4.5. If Λ is singular, then set $\Lambda = I$.

We keep track of the progress of the procedure by computing $\varphi(X^*, Q^*) = \|X^* - ZQ^*\|_F$ after every step and checking that X^* or $\varphi(X^*, Q^*)$ stops changing, whichever comes first. We observed that after a small number of steps, up to machine precision, $\varphi(X^*, Q^*)$ stops decreasing, and when this occurs the procedure halts (we also set a maximum number of steps in case $\varphi(X^*, Q^*)$ decreases for a very long time). Moreover, looking for $Q = R\Lambda$ where $R \in \mathbf{O}(K)$ and Λ is obtained using the method of Proposition 4.5 speeds up the convergence and yields a better discrete solution X.

The process of searching for X and Q has an illuminating geometric interpretation in terms of graph drawings. We may assume that the entries in the discrete solution X are 0 or 1. Then the rows of the discrete solutions X correspond to the tips of the unit vectors along the coordinate axes in $\mathbb{R}^K$. Every axis contains at least such a point, and the multiplicity of the point along the jth axis is the number of nodes in the jth block of the partition. Similarly, the rows of Z are the nodes of a graph drawing of the weighted graph (V, W). Multiplying Z on the right by a $K \times K$ matrix Q (obtaining ZQ) is equivalent to multiplying $Z^\top$ on the left by $Q^\top$ (obtaining $Q^\top Z^\top$). This means that the points in $\mathbb{R}^K$ representing the rows of ZQ are obtained by applying the linear transformation $Q^\top$ to the columns of $Z^\top$. Thus, ZR amounts to applying the rigid motion $R^\top$ to the graph drawing Z, and $Z\Lambda$ (where Λ is

a diagonal invertible matrix) amounts to stretching or shrinking the graph drawing Z in the directions of the axes.

Then, in step 2 (PODR), we are trying to deform the graph drawing given by Z using a linear map $(R\Lambda)^\top$, so that the deformed graph drawing $ZR\Lambda$ is as close as possible to X (in the sense that $\|X - ZR\Lambda\|_F$ is minimized).

In step 1 (PODX), we are trying to approximate the deformed graph drawing $ZR\Lambda$ by a discrete graph drawing X (whose nodes are the tips of the unit vectors), so that $\|X - ZR\Lambda\|_F$ is minimized.

If we are willing to give up the requirement that the deformed Z is still a solution of problem $(*_1)$, we have quite a bit of freedom in step 2. For example, we may allow normalizing the rows. This seems reasonable to obtain an initial transformation Q. However, we feel uncomfortable in allowing intermediate deformed Z that are not solutions of $(*_1)$ during the iteration process. This point should be investigated further.

In some sense, we have less freedom in step 1, since the ith row of $ZR\Lambda$ is assigned to the jth unit vector iff the index of the leftmost largest coordinate of this row is j. If some axis has not been assigned any row of R, then we reallocate one of the points on an axis with a maximum number of points.

Figure 4.5 shows a graph (on the left) and the graph drawings X and $Z * R$ obtained by applying our method for three clusters. The rows of X are represented by the red points along the axes, and the rows of $Z * R$ by the green points (on the right). The original vertices corresponding to the rows of Z are represented in blue. We can see how the two red points correspond to an edge, the three red points correspond to a triangle, and the four red points to a quadrangle. These constitute the clusters.

It remains to initialize Q^* to start the process, and then steps (1) and (2) are iterated, starting with step (1). Actually, what we really need is a "good" initial X^*, but to find it, we need an initial R^*.

Method 1. One method is to use an orthogonal matrix denoted R_1, such that distinct columns of ZR_1 are simultaneously orthogonal and D-orthogonal. The matrix R_1 can be found by diagonalizing $Z^\top Z$ as $Z^\top Z = R_1 \Sigma R_1^\top$, as we explained at the end of Section 4.3. We write $Z_2 = ZR_1$.

Method 2. The method advocated by Yu [23] is to pick K rows of Z that are as orthogonal to each other as possible and to make a matrix R whose columns consist of these rows normalized to have unit length. The intuition behind this method is that if a continuous solution Z can be sent close to a discrete solution X by a rigid motion, then many rows of Z viewed as vectors in $\mathbb{R}^K$ should be nearly orthogonal. This way, ZR should contain at least K rows well aligned with the canonical basis vectors, and these rows are good candidates for some of the rows of the discrete solution X.

The algorithm given in Yu [23] needs a small correction, because rows are not removed from Z when they are added to R, which may cause the same row to be added several times to R.

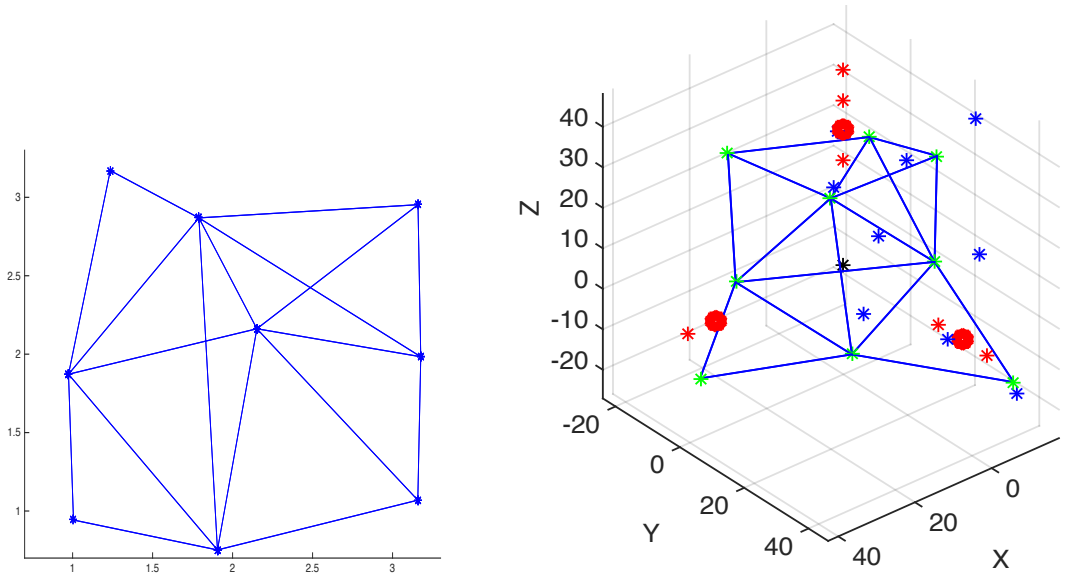

Figure 4.5: A graph and its drawing to find 3 clusters.

Given the $N \times K$ matrix Z (whose columns all have the same norm), we compute a matrix R whose columns are certain rows of Z. We use a vector $c \in \mathbb{R}^N$ to keep track of the inner products of all rows of Z with the columns $R^1, \ldots, R^{k-1}$ that have been constructed so far, and initially when $k = 1$, we set $c = 0$.

The first column R^1 of R is any chosen row of Z.

Next, for $k = 2, \ldots, K$, we compute all the inner products of R^{k-1} with all rows in Z, which are recorded in the vector ZR^{k-1}, and we update c as follows:

$$c = c + \mathtt{abs}(ZR^{k-1}).$$

We take the absolute values of the entries in ZR^{k-1} so that the ith entry in c is a score of how orthogonal is the ith row of Z to $R^1, \ldots, R^{k-1}$. Then, we choose R^k as any row Z_i of Z for which c_i is minimal (the customary (and ambiguous) $i = \arg\min c$), and we delete this row from Z. The process is repeated (with the updated Z) until $k = K$.

At the end of the above process, we normalize the columns of R, to obtain a matrix that we denote R_2.

After some experimentation, we found that to obtain a better initial X^*, it is may desirable to start from a variant of the continuous solution Z obtained by solving problem $(*_2)$. We have implemented three methods.

1. We attempt to rescale the columns of Z by some diagonal invertible matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_K)$, so that the rows of $Z\Lambda$ sum to 1 as much as possible in the least-squares sense. Since the vector of sums of rows of $Z\Lambda$ is $Z\Lambda \mathbf{1}_K = Z\lambda$, with $\lambda^\top =$

$(\lambda_1, \ldots, \lambda_K)$, the least-squares problem is to minimize

$$\|Z\lambda - \mathbf{1}_N\|_2^2,$$

and since Z has rank K, the solution is $\lambda = (Z^\top Z)^{-1} Z^\top \mathbf{1}_N$, and thus,

$$\Lambda = \mathrm{diag}((Z^\top Z)^{-1} Z^\top \mathbf{1}_N).$$

The matrix Λ is singular if some of the columns of Z sum to 0. This happens for regular graphs, where the degree matrix is a multiple of the identity. There are also cases where some of the λ_j are very small, so we use a tolerance factor to prevent this, and in case of failure, we set $\Lambda = I$. In case of failure, we may also use ZR_1 instead of Z, where R_1 is the orthogonal matrix that makes ZR_1 both D-orthogonal and orthogonal.

2. We attempt to rescale the columns of Z by some diagonal invertible matrix $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_K)$, so that the rows of $Z\Lambda$ have unit length as much as possible in the least-squares sense. Since the square-norm of the ith row of $Z\Lambda$ is

$$\sum_{j=1}^{K} z_{ij}^2 \lambda_j^2,$$

if we write $Z \circ Z$ for the matrix (z_{ij}^2) of square entries of elements in Z (the Hadamard product of Z with itself), the least-squares problem is to mimimize

$$\left\|Z \circ Z\lambda^2 - \mathbf{1}_N\right\|_2^2,$$

where $(\lambda^2)^\top = (\lambda_1^2, \ldots, \lambda_K^2)$. The matrix $Z \circ Z$ may not have rank K, so the least-squares solution for λ^2 is given by the pseudo-inverse of $Z \circ Z$, as

$$\lambda^2 = (Z \circ Z)^+ \mathbf{1}_N.$$

There is no guarantee that the vector on the right-hand side has all positive entries, so the method may fail. It may also fail when some of the λ_j are very small. We use a tolerance factor to prevent this, and in case of failure, we set $\Lambda = I$.

3. We use a method more drastic than (2), which consists in normalizing the rows of Z. Thus, we form the matrix

$$NZ = \mathrm{diag}((ZZ^\top)_{11}^{-1/2}, \ldots, (ZZ^\top)_{NN}^{-1/2}),$$

and we return $NZ * Z$. Unlike the methods used in (1) and (2), this method does not guarantee that $NZ * Z$ is a solution of problem $(*_1)$. However, since the rows of Z can be interpreted as vectors in $\mathbb{R}^K$ that should align as much as possible with the canonical basis vectors of $\mathbb{R}^K$, this method makes sense as a way to come closer to a discrete solution. In fact, we found that it does well in most cases.

We implemented a computer program that prompts the user for various options. To avoid confusion, let us denote the original solution of problem $(*_2)$ by Z_1, and let $Z_2 = Z_1 R_1$, as obtained by initialization method 1. The four options are:

1. Use the original solution Z_1 of problem $(*_2)$, as well as Z_2.
2. Apply method 1 to Z_1 and Z_2.
3. Apply method 2 to Z_1 and Z_2.
4. Apply method 3 to Z_1 and Z_2.

Then, for each of these options, if we denote by $Zinit_1$ and $Zinit_2$ the solutions returned by the method, our program computes initial solutions X_1, X_2, X_3, X_4 as follows:

1. Use $Zinit_1$ and $R = I$.
2. Use $Zinit_1$ and $R = R2a$, the matrix given by initialization method 2.
3. Use $Zinit_2$ and $R = I$.
4. Use $Zinit_2$ and $R = R2b$, the matrix given by initialization method 2.

After this, the program picks the discrete solution $X = X_i$ which corresponds to the minimum of

$$\|X1 - Zinit1\|\,,\ \|X2 - Zinit1 * R2a\|\,,\ \|X3 - Zinit2\|\,,\ \|X4 - Zinit2 * R2b\|\,.$$

Our experience is that options (3) and (4) tend to give better results. However, it is harder to say whether any of the X_i does a better job than the others, although (2) and (4) seem to do slightly better than (1) and (3). We also give the user the option in step PODR to only compute R and set $\Lambda = I$. It appears that the more general method is hardly more expansive (because finding Λ is cheap) and always gives better results.

We also found that we obtain better results if we rescale Z (and X) so that$\|Z\|_F = 100$.

If we apply the method (using method 3 to find the initial R) to the graph associated with the the matrix W_1 shown in Figure 4.6 for $K = 4$ clusters, the algorithm converges in 3 steps and we find the clusters shown in Figure 4.7.

The solution Z of the relaxed problem is

$$Z = \begin{pmatrix} -21.3146 & -0.0000 & 19.4684 & -15.4303 \\ -4.1289 & 0.0000 & 16.7503 & -15.4303 \\ -21.3146 & 32.7327 & -19.4684 & -15.4303 \\ -4.1289 & -0.0000 & 16.7503 & -15.4303 \\ 19.7150 & 0.0000 & 9.3547 & -15.4303 \\ -4.1289 & 23.1455 & -16.7503 & -15.4303 \\ -21.3146 & -32.7327 & -19.4684 & -15.4303 \\ -4.1289 & -23.1455 & -16.7503 & -15.4303 \\ 19.7150 & -0.0000 & -9.3547 & -15.4303 \end{pmatrix}.$$

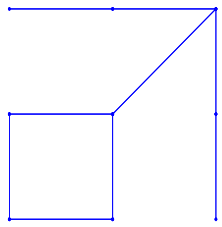

Figure 4.6: Underlying graph of the matrix W_1.

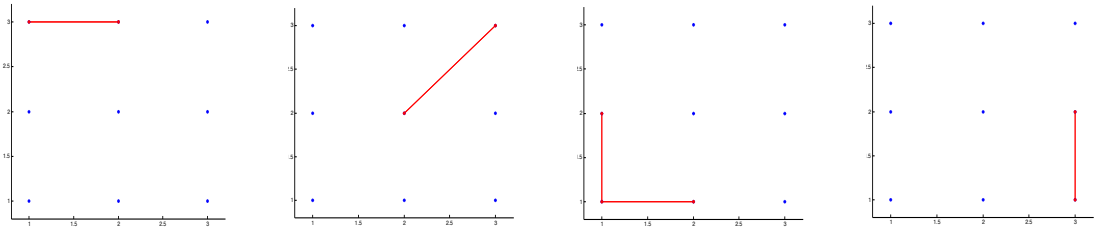

Figure 4.7: Four blocks of a normalized cut for the graph associated with W_1 .

We find the following sequence for $Q, Z * Q, X$:

$$Q = \begin{pmatrix} 0 & 0.6109 & -0.3446 & -0.7128 \\ -1.0000 & 0.0000 & 0.0000 & -0.0000 \\ 0.0000 & 0.5724 & 0.8142 & 0.0969 \\ -0.0000 & 0.5470 & -0.4672 & 0.6947 \end{pmatrix},$$

which is the initial Q obtained by method 1;

$$Z * Q = \begin{pmatrix} 0.0000 & -10.3162 & 30.4065 & 6.3600 \\ 0.0000 & -1.3742 & 22.2703 & -6.1531 \\ -32.7327 & -32.6044 & -1.2967 & 2.5884 \\ 0.0000 & -1.3742 & 22.2703 & -6.1531 \\ 0.0000 & 8.9576 & 8.0309 & -23.8653 \\ -23.1455 & -20.5505 & -5.0065 & -9.3982 \\ 32.7327 & -32.6044 & -1.2967 & 2.5884 \\ 23.1455 & -20.5505 & -5.0065 & -9.3982 \\ -0.0000 & -1.7520 & -7.2027 & -25.6776 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix};$$

$$Q = \begin{pmatrix} -0.0803 & 0.8633 & -0.4518 & -0.2102 \\ -0.6485 & 0.1929 & 0.1482 & 0.7213 \\ -0.5424 & 0.0876 & 0.5546 & -0.6250 \\ -0.5281 & -0.4581 & -0.6829 & -0.2119 \end{pmatrix}$$

$$Z * Q = \begin{pmatrix} -0.6994 & -9.6267 & 30.9638 & -4.4169 \\ -0.6051 & 4.9713 & 21.6922 & -6.3311 \\ -0.8081 & -6.7218 & 14.2223 & 43.5287 \\ -0.6051 & 4.9713 & 21.6922 & -6.3311 \\ 1.4913 & 24.9075 & 6.8186 & -6.7218 \\ 2.5548 & 6.5028 & 6.5445 & 31.3015 \\ 41.6456 & -19.3507 & 4.5190 & -3.6915 \\ 32.5742 & -2.4272 & -0.3168 & -2.0882 \\ 11.6387 & 23.2692 & -3.5570 & 4.9716 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix};$$

$$Q = \begin{pmatrix} -0.3201 & 0.7992 & -0.3953 & -0.3201 \\ -0.7071 & -0.0000 & 0.0000 & 0.7071 \\ -0.4914 & -0.0385 & 0.7181 & -0.4914 \\ -0.3951 & -0.5998 & -0.5728 & -0.3951 \end{pmatrix}$$

$$Z * Q = \begin{pmatrix} 3.3532 & -8.5296 & 31.2440 & 3.3532 \\ -0.8129 & 5.3103 & 22.4987 & -0.8129 \\ -0.6599 & -7.0310 & 3.2844 & 45.6311 \\ -0.8129 & 5.3103 & 22.4987 & -0.8129 \\ -4.8123 & 24.6517 & 7.7629 & -4.8123 \\ -0.7181 & 6.5997 & -1.5571 & 32.0146 \\ 45.6311 & -7.0310 & 3.2844 & -0.6599 \\ 32.0146 & 6.5997 & -1.5571 & -0.7181 \\ 4.3810 & 25.3718 & -5.6719 & 4.3810 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

During the next round, the exact same matrices are obtained and the algorithm stops. Comparison of the matrices $Z * Q$ and X makes it clear that X is obtained from $Z * Q$ by retaining on every row the leftmost largest value and setting the others to 0 (non-maximum supression).

In this example, the columns of all X were nonzero, but this may happen, for example when we apply the algorithm to the graph of Figure 4.6 to find $K = 5$ clusters shown in Figure 4.8.

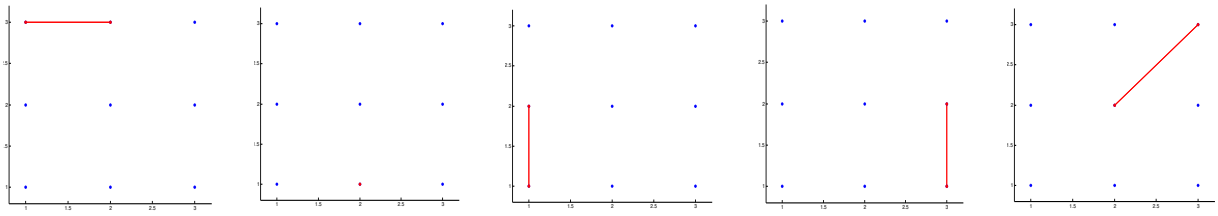

Figure 4.8: Five blocks of a normalized cut for the graph associated with W_1 .

We find that the initial value for $Z * Q$ is

$$Z * Q = \begin{pmatrix} -5.7716 & -27.5934 & 0.0000 & -9.3618 & -0.0000 \\ 5.5839 & -20.2099 & -29.7044 & -1.2471 & -0.0000 \\ -2.3489 & 1.1767 & -0.0000 & -29.5880 & -29.7044 \\ 5.5839 & -20.2099 & 29.7044 & -1.2471 & 0.0000 \\ 21.6574 & -7.2879 & 0.0000 & 8.1289 & 0.0000 \\ 8.5287 & 4.5433 & -0.0000 & -18.6493 & -21.0042 \\ -2.3489 & 1.1767 & -0.0000 & -29.5880 & 29.7044 \\ 8.5287 & 4.5433 & -0.0000 & -18.6493 & 21.0042 \\ 23.3020 & 6.5363 & -0.0000 & -1.5900 & -0.0000 \end{pmatrix}.$$

The matrix $X1$ given by the above method in which we pick the leftmost largest entry on every row has a fourth row equal to 0. The matrix $X1$ is repaired by migrating a 1 from the second entry of the first column, which contains the largest number of 1's, yielding the matrix $X2$; see below.

$$X1 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad X2 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Chapter 5

Signed Graphs

5.1 Signed Graphs and Signed Laplacians

Intuitively, in a weighted graph, an edge with a positive weight denotes similarity or proximity of its endpoints. For many reasons, it is desirable to allow edges labeled with negative weights, the intuition being that a negative weight indicates dissimilarity or distance.

Weighted graphs for which the weight matrix is a symmetric matrix in which negative and positive entries are allowed are called *signed graphs*. Such graphs (with weights $(-1, 0, +1)$) were introduced as early as 1953 by Harary [12], to model social relations involving disliking, indifference, and liking. The problem of clustering the nodes of a signed graph arises naturally as a generalization of the clustering problem for weighted graphs. From our perspective, we would like to know whether clustering using normalized cuts can be extended to signed graphs.

Given a signed graph $G = (V, W)$ (where W is a symmetric matrix with zero diagonal entries), the *underlying graph* of G is the graph with node set V and set of (undirected) edges $E = \{\{v_i, v_j\} \mid w_{ij} \neq 0\}$.

The first obstacle is that the degree matrix may now contain zero or negative entries. As a consequence, the Laplacian L may no longer be positive semidefinite, and worse, $D^{-1/2}$ may not exist.

A simple remedy is to use the absolute values of the weights in the degree matrix! This idea applied to signed graph with weights $(-1, 0, 1)$ occurs in Hou [14]. Kolluri, Shewchuk and O'Brien [15] take the natural step of using absolute values of weights in the degree matrix in their original work on surface reconstruction from noisy point clouds. Given a Delaunay tetrahedralization, they build a graph with positive and negative edges and use the normalized cut method for two clusters to decide which tetrahedra are inside or outside the original object. The triangulated surface (called the *eigencrust*) consists of the triangles where an inside and an outside tetrahedron meet. The authors state that the Lapacians arising from such graphs are always positive definite, which is not quite correct since this is only true for unbalanced graphs (see Section 5.3). Kunegis et al. [16] appear to be the

first to make a systematic study of spectral methods applied to signed graphs. In fact, many results in this section originate from Kunegis et al. [16]. However, it should be noted that only 2-clustering is considered in the above papers.

As we will see, the trick of using absolute values of weights in the degree matrix allows the whole machinery that we have presented to be used to attack the problem of clustering signed graphs using normalized cuts. This requires a modification of the notion of normalized cut. This new notion it is quite reasonable, as we will see shortly.

If (V, W) is a signed graph, where W is an $m \times m$ symmetric matrix with zero diagonal entries and with the other entries $w_{ij} \in \mathbb{R}$ arbitrary, for any node $v_i \in V$, the *signed degree* of v_i is defined as

$$\overline{d}_i = \overline{d}(v_i) = \sum_{j=1}^{m} |w_{ij}|,$$

and the *signed degree matrix* $\overline{D}$ as

$$\overline{D} = \mathrm{diag}(\overline{d}(v_1), \ldots, \overline{d}(v_m)).$$

For any subset A of the set of nodes V, let

$$\mathrm{vol}(A) = \sum_{v_i \in A} \overline{d}_i = \sum_{v_i \in A} \sum_{j=1}^{m} |w_{ij}|.$$

For any two subsets A and B of V, define $\mathrm{links}^+(A, B)$, $\mathrm{links}^-(A, B)$, and $\mathrm{cut}(A, \overline{A})$ by

$$\begin{aligned}
\mathrm{links}^+(A, B) &= \sum_{\substack{v_i \in A, v_j \in B \\ w_{ij} > 0}} w_{ij} \\
\mathrm{links}^-(A, B) &= \sum_{\substack{v_i \in A, v_j \in B \\ w_{ij} < 0}} -w_{ij} \\
\mathrm{cut}(A, \overline{A}) &= \sum_{\substack{v_i \in A, v_j \in \overline{A} \\ w_{ij} \neq 0}} |w_{ij}|.
\end{aligned}$$

Note that $\mathrm{links}^+(A, B) = \mathrm{links}^+(B, A)$, $\mathrm{links}^-(A, B) = \mathrm{links}^-(B, A)$, and

$$\mathrm{cut}(A, \overline{A}) = \mathrm{links}^+(A, \overline{A}) + \mathrm{links}^-(A, \overline{A}).$$

Then, the *signed Laplacian* $\overline{L}$ is defined by

$$\overline{L} = \overline{D} - W,$$

and its normalized version $\overline{L}_{\mathrm{sym}}$ by

$$\overline{L}_{\mathrm{sym}} = \overline{D}^{-1/2} \overline{L} \overline{D}^{-1/2} = I - \overline{D}^{-1/2} W \overline{D}^{-1/2}.$$

For a graph without isolated vertices, we have $\overline{d}(v_i) > 0$ for $i = 1, \ldots, m$, so $\overline{D}^{-1/2}$ is well defined.

The signed Laplacian is symmetric positive semidefinite. As for the Laplacian of a weight matrix (with nonnegative entries), this can be shown in two ways. The first method consists in defining a notion of incidence matrix for a signed graph, and appears in Hou [14].

Definition 5.1. Given a signed graph $G = (V, W)$, with $V = \{v_1, \ldots, v_m\}$, if $\{e_1, \ldots, e_n\}$ are the edges of the underlying graph of G (recall that $\{v_i, v_j\}$ is an edge of this graph iff $w_{ij} \neq 0$), for any oriented graph G^σ obtained by giving an orientation to the underlying graph of G, the *incidence matrix* B^σ of G^σ is the $m \times n$ matrix whose entries $b_{i\,j}$ are given by

$$b_{i\,j} = \begin{cases} +\sqrt{w_{ij}} & \text{if } w_{ij} > 0 \text{ and } s(e_j) = v_i \\ -\sqrt{w_{ij}} & \text{if } w_{ij} > 0 \text{ and } t(e_j) = v_i \\ \sqrt{-w_{ij}} & \text{if } w_{ij} < 0 \text{ and } (s(e_j) = v_i \text{ or } t(e_j) = v_i) \\ 0 & \text{otherwise.} \end{cases}$$

Then, we have the following proposition whose proof is easily adapted from the proof of Proposition 2.2.

Proposition 5.1. *Given any signed graph $G = (V, W)$ with $V = \{v_1, \ldots, v_m\}$, if B^σ is the incidence matrix of any oriented graph G^σ obtained from the underlying graph of G and $\overline{D}$ is the signed degree matrix of W, then*

$$B^\sigma (B^\sigma)^\top = \overline{D} - W = \overline{L}.$$

Consequently, $B^\sigma (B^\sigma)^\top$ is independent of the orientation of the underlying graph of G and $\overline{L} = \overline{D} - W$ is symmetric and positive semidefinite; that is, the eigenvalues of $\overline{L} = \overline{D} - W$ are real and nonnegative.

Another way to prove that $\overline{L}$ is positive semidefinite is to evaluate the quadratic form $x^\top \overline{L} x$. We will need this computation to figure out what is the new notion of normalized cut. For any real $\lambda \in \mathbb{R}$, define $\mathrm{sgn}(\lambda)$ by

$$\mathrm{sgn}(\lambda) = \begin{cases} +1 & \text{if } \lambda > 0 \\ -1 & \text{if } \lambda < 0 \\ 0 & \text{if } \lambda = 0. \end{cases}$$

Proposition 5.2. *For any $m \times m$ symmetric matrix $W = (w_{ij})$, if we let $\overline{L} = \overline{D} - W$ where $\overline{D}$ is the signed degree matrix associated with W, then we have*

$$x^\top \overline{L} x = \frac{1}{2} \sum_{i,j=1}^{m} |w_{ij}| (x_i - \mathrm{sgn}(w_{ij}) x_j)^2 \quad \text{for all } x \in \mathbb{R}^m.$$

Consequently, $\overline{L}$ is positive semidefinite.

Proof. We have

$$\begin{aligned}
x^\top \overline{L} x &= x^\top \overline{D} x - x^\top W x \\
&= \sum_{i=1}^m \overline{d}_i x_i^2 - \sum_{i,j=1}^m w_{ij} x_i x_j \\
&= \sum_{i,j=1}^m (|w_{ij}| x_i^2 - w_{ij} x_i x_j) \\
&= \sum_{i,j=1}^m (|w_{ij}| (x_i^2 - \mathrm{sgn}(w_{ij}) x_i x_j) \\
&= \frac{1}{2} \left(\sum_{i,j=1}^m |w_{ij}| (x_i^2 - 2\mathrm{sgn}(w_{ij}) x_i x_j + x_j^2) \right) \\
&= \frac{1}{2} \sum_{i,j=1}^m |w_{ij}| (x_i - \mathrm{sgn}(w_{ij}) x_j)^2,
\end{aligned}$$

and this quantity is nonnegative. □

5.2 Signed Normalized Cuts

As in Section 4.3, given a partition of V into K clusters $(A_1, \ldots, A_K)$, if we represent the jth block of this partition by a vector X^j such that

$$X_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ 0 & \text{if } v_i \notin A_j, \end{cases}$$

for some $a_j \neq 0$, then we have the following result.

Proposition 5.3. *For any vector X^j representing the jth block of a partition $(A_1, \ldots, A_K)$ of V, we have*

$$(X^j)^\top \overline{L} X^j = a_j^2 (\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)).$$

Proof. Using Proposition 5.2, we have

$$(X^j)^\top \overline{L} X^j = \frac{1}{2} \sum_{i,k=1}^m |w_{ik}| (X_i^j - \mathrm{sgn}(w_{ik}) X_k^j)^2.$$

The sum on the righthand side splits into four parts:

(1) $S_1 = \frac{1}{2} \sum_{i,k \in A_j} |w_{ik}| (X_i^j - \mathrm{sgn}(w_{ik}) X_k^j)^2$. In this case, $X_i^j = X_k^j = a_j$, so only negative edges have a nonzero contribution, and we have

$$S_1 = \frac{1}{2} \sum_{i,k \in A_j, w_{ik} < 0} |w_{ik}| (a_j + a_j)^2 = 2a_j^2 \mathrm{links}^-(A_j, A_j).$$

(2) $S_2 = \frac{1}{2}\sum_{i\in A_j, k\in\overline{A_j}} |w_{ik}|(X_i^j - \mathrm{sgn}(w_{ik})X_k^j)^2$. In this case, $X_i^j = a_j$ and $X_k^j = 0$, so

$$S_2 = \frac{1}{2}a_j^2 \sum_{i\in A_j, k\in\overline{A_j}} |w_{ik}| = \frac{1}{2}a_j^2 \mathrm{cut}(A_j, \overline{A_j}).$$

(3) $S_3 = \frac{1}{2}\sum_{i\in\overline{A_j}, k\in A_j} |w_{ik}|(X_i^j - \mathrm{sgn}(w_{ik})X_k^j)^2$. In this case, $X_i^j = 0$ and $X_k^j = a_j$, so

$$S_3 = \frac{1}{2}a_j^2 \sum_{i\in\overline{A_j}, k\in A_j} |w_{ik}| = \frac{1}{2}a_j^2 \mathrm{cut}(\overline{A_j}, A_j) = \frac{1}{2}a_j^2 \mathrm{cut}(A_j, \overline{A_j}).$$

(4)

$S_4 = \frac{1}{2}\sum_{i,k\in\overline{A_j}} |w_{ik}|(X_i^j - \mathrm{sgn}(w_{ik})X_k^j)^2$. In this case, $X_i^j = X_k^j = 0$, so

$$S_4 = 0.$$

In summary,

$$(X^j)^\top \overline{L} X^j = S_1 + S_2 + S_3 + S_4 = 2a_j^2 \mathrm{links}^-(A_j, A_j) + a_j^2 \mathrm{cut}(A_j, \overline{A_j}),$$

as claimed. □

Since with the revised definition of $\mathrm{vol}(A_j)$, we also have

$$(X^j)^\top \overline{D} X^j = a_j^2 \sum_{v_i\in A_j} \overline{d}_i = a_j^2 \mathrm{vol}(A_j),$$

we deduce that

$$\frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j} = \frac{\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)}{\mathrm{vol}(A_j)}.$$

The calculations of the previous paragraph suggest the following definition.

Definition 5.2. The *signed normalized cut* $\mathrm{sNcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ is defined as

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{\mathrm{vol}(A_j)} + 2\sum_{j=1}^{K} \frac{\mathrm{links}^-(A_j, A_j)}{\mathrm{vol}(A_j)}.$$

Remark: Kunegis et al. [16] deal with a different notion of cut, namely ratio cut (in which $\mathrm{vol}(A)$ is replaced by the size $|A|$ of A), and only for two clusters. In this case, by a clever choice of indicator vector, they obtain a notion of signed cut that only takes into account the positive edges between A and $\overline{A}$, and the negative edges among nodes in A and nodes in $\overline{A}$. This trick does not seem to generalize to more than two clusters, and this is why we

use our representation for partitions. Our definition of a signed normalized cut appears to be novel.

Based on previous computations, we have

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j}.$$

where X is the $N \times K$ matrix whose jth column is X^j. Therefore, this is the same problem as in Chapter 4, with L replaced by $\overline{L}$ and D replaced by $\overline{D}$.

Observe that minimizing $\mathrm{sNcut}(A_1, \ldots, A_K)$ amounts to minimizing the number of positive and negative edges between clusters, and also minimizing the number of negative edges within clusters. This second minimization captures the intuition that nodes connected by a negative edge should not be together (they do not "like" each other; they should be far from each other).

The K-clustering problem for signed graphs is related but not equivalent to another problem known as *correlation clustering*. In correlation clustering, in our terminology and notation, given a graph $G = (V, W)$ with positively and negatively weighted edges, one seeks a clustering of V that minimizes the sum $\mathrm{links}^-(A_j, A_j)$ of the absolute values of the negative weights of the edges within each cluster A_j, and minimizes the sum $\mathrm{links}^+(A_j, \overline{A}_j)$ of the positive weights of the edges between distinct clusters. In contrast to K-clustering, the number K of clusters is not given in advance, and there is no normalization with respect to size of volume. Furthermore, in correlation clustering, only the contribution $\mathrm{links}^+(A_j, \overline{A}_j)$ of positively weighted edges is minimized, but our method only allows us to minimize $\mathrm{cut}(A_j, \overline{A}_j)$, which also takes into account negatively weighted edges between distinct clusters. Correlation clustering was first introduced and studied for complete graphs by Bansal, Blum and Chawla [1]. They prove that this problem is NP-complete and give several approximation algorithms, including a PTAS for maximizing agreement. Demaine and Immorlica [5] consider the same problem for arbitrary weighted graphs, and they give an $O(\log n)$-approximation algorithm based on linear programming. Since correlation clustering does not assume that K is given and not not include nomalization by size or volume, it is not clear whether algorithms for correlation clustering can be applied to normalized K-clustering, and conversely.

5.3 Balanced Graphs

Since

$$\mathrm{sNcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top \overline{D} X^j},$$

the whole machinery of Sections 4.3 and 4.5 can be applied with D replaced by $\overline{D}$ and L replaced by $\overline{L}$. However, there is a new phenomenon, which is that $\overline{L}$ may be positive

definite. As a consequence, $\mathbf{1}$ is not always an eigenvector of $\overline{L}$. As observed by Kunegis et al. [16], it is also possible to characterize for which signed graphs the Laplacian $\overline{L}$ is positive definite. Such graphs are "cousins" of bipartite graphs and were introduced by Harary [12]. Since a graph is the union of its connected components, we restrict ourselves to connected graphs.

Definition 5.3. Given a signed graph $G = (V, W)$ with negative weights whose underlying graph is connected, we say that G is *balanced* if there is a partition of its set of nodes V into two blocks V_1 and V_2 such that all positive edges connect nodes within V_1 or V_2, and negative edges connect nodes between V_1 and V_2.

An example of a balanced graph is shown in Figure 5.1 on the left, in which positive edges are colored green and negative edges are colored red. This graph admits the partition

$$(\{v_1, v_2, v_4, v_7, v_8\}, \{v_3, v_5, v_6, v_9\}).$$

On the other hand, the graph shown on the right contains the cycle $(v_2, v_3, v_6, v_5, v_4, v_2)$ with an odd number of negative edges (3), and thus is not balanced.

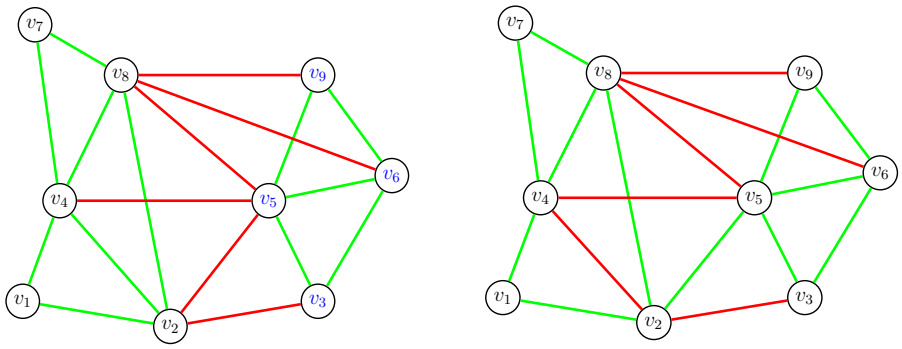

Figure 5.1: A balanced signed graph G_1 (left). An unbalanced signed graph G_2 (right).

Observe that if we delete all positive edges in a balanced graph, then the resulting graph is bipartite. Then, it is not surprising that connected balanced graphs can be characterized as signed graphs in which every cycle has an even number of negative edges. This is analogous to the characterization of a connected bipartite graph as a graph in which every cycle has even length. The following proposition was first proved by Harary [12]. We give a more direct proof.

Proposition 5.4. *If $G = (V, W)$ is a connected signed graph with negative weights, then G is balanced iff every cycle contains an even number of negative edges.*

Proof. If G is balanced, then every cycle must switch from a node in V_1 to a node in V_2 (or from a node in V_2 to a node in V_1) an even number of times. Therefore, it contains an even number of negative edges.

Conversely, assume that G contains no cycle with an odd number of negative edges. Since G is connected, pick some some v_0 in V, and let V_1 be the set of node reachable from v_0 by a path with an odd number of negative edges, and let V_2 be the set of node reachable from v_0 by a path with an even number of negative edges. Clearly, (V_1, V_2) is a partition of V. Assume that there is a negative edge $\{u, v\}$ between two nodes within V_1 (or V_2). Then, using the paths from v_0 to u and v, where the parity of the number of negative edges is the same, we would obtain a cycle with an odd number of negative edges, a contradiction. Therefore, edges between nodes in V_1 (or V_2) are positive, and negative edges connect nodes in V_1 and V_2. □

We can also detect whether a connected signed graph is balanced in terms of the kernel of the transpose of any of its incidence matrices.

Proposition 5.5. *If $G = (V, W)$ is a connected signed graph with negative weights and with m nodes, for any orientation of its underlying graph, let B be the corresponding incidence matrix. The underlying graph of G is balanced iff* $\mathrm{rank}(B) = m - 1$. *Furthermore, if G is balanced, then there is a vector u with $u_i \in \{-1, 1\}$ such that $B^\top u = 0$, and the sets of nodes $V_1 = \{v_i \mid u_i = -1\}$ and $V_2 = \{v_i \mid u_i = +1\}$ form a partition of V for which G is balanced.*

Proof. Assume that $\mathrm{rank}(B) = m - 1$; this implies that $\mathrm{Ker}\,(B^\top) \neq (0)$. For any $u \neq 0$, we have $B^\top u = 0$ iff $u^\top B = 0$ iff u is orthogonal to every column of B. By definition of B, we have

$$u_i = \mathrm{sgn}(w_{ij}) u_j$$

iff there is an edge between v_i and v_j.

Pick node v_1 in V and define V_1 and V_2 as in the proof of Proposition 5.4. The above equation shows that u has the same value on nodes connected by a path with an even number of negative edges, and opposite values on nodes connected by a path with an odd number of negative edges. Since V_1 consists of all nodes connected to v_1 by a path with an odd number of negative edges and V_2 consists of all nodes connected to v_1 by a path with an even number of negative edges, it follows that u has the same value $c = u_1$ on all nodes in V_1, and the value $-c$ on all nodes in V_2. Then, there is no negative edge between any two nodes in V_1 (or V_2), since otherwise u would take opposite values on theses two nodes, contrary to the fact that u has a constant value on V_1 (and V_2). This implies that (V_1, V_2) is a partition of V making G a balanced graph.

Conversely, if G is balanced, then there is a partition (V_1, V_2) of V such that positive edges connect nodes within V_1 or V_2, and negative edges connect nodes between V_1 and V_2. Then, if u is the vector with $u_i \in \{-1, 1\}$ defined so that $u_i = +1$ iff $v_i \in V_1$ and $u_i = -1$ iff $v_i \in V_2$, we have

$$u_i = \mathrm{sgn}(w_{ij}) u_j,$$

and so $B^\top u = 0$, which shows that $u \in \mathrm{Ker}\,(B^\top)$. Furthermore, the argument in the first part of the proof shows that every vector in $\mathrm{Ker}\,(B^\top)$ must have the same value c on all

nodes in V_1, and the value $-c$ on all nodes in V_2, so it must be a multiple of the vector u given by $u_i = +1$ iff $v_i \in V_1$ and $u_i = -1$ iff $v_i \in V_2$. Therefore, $\dim(\mathrm{Ker}\,(B^\top)) = 1$, and $\mathrm{rank} = m - 1$. The third part of the proposition has already been shown. □

Remark: A simple modification of the proof of Proposition 5.5 shows that if there are c_1 components containing only positive edges, c_2 components that are balanced graphs, and c_3 components that are not balanced (and contain some negative edge), then

$$c_1 + c_2 = m - \mathrm{rank}(B).$$

Since by Proposition 5.1 we have $\overline{L} = BB^\top$ for any incidence matrix B associated with an orientation of the underlying graph of G, we obtain the following important result (which is proved differently in Kunegis et al. [16]).

Theorem 5.6. *The signed Laplacian $\overline{L}$ of a connected signed graph G is positive definite iff G is not balanced (possesses some cycle with an odd number of negative edges).*

If $G = (V, W)$ is a balanced graph, then there is a partition (V_1, V_2) of V such that for every edge $\{v_i, v_j\}$, if $w_{ij} > 0$, then $v_i, v_j \in V_1$ or $v_i, v_j \in V_2$, and if $w_{ij} < 0$, then $v_i \in V_1$ and $v_j \in V_2$. It follows that if we define the vector x such that $x_i = +1$ iff $v_i \in V_1$ and $x_i = -1$ iff $v_i \in V_2$, then for every edge $\{v_i, v_j\}$ we have

$$\mathrm{sgn}(w_{ij}) = x_i x_j.$$

We call x a *bipartition* of V.

The signed Laplacian of the balanced graph G_1 is given by

$$\overline{L}_1 = \begin{pmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 5 & 1 & -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 3 & 0 & -1 & -1 & 0 & 0 & 0 \\ -1 & -1 & 0 & 5 & 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 1 & 6 & -1 & 0 & 1 & -1 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 2 & -1 & 0 \\ 0 & -1 & 0 & -1 & 1 & 1 & -1 & 6 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 1 & 3 \end{pmatrix}$$

Using `Matlab`, we find that its eigenvalues are

$$0,\ 1.4790,\ 1.7513,\ 2.7883,\ 4.3570,\ 4.8815,\ 6.2158,\ 7.2159,\ 7.3112.$$

The eigenvector corresponding to the eigenvalue 0 is

$$(0.3333,\ 0.3333,\ -0.3333,\ 0.3333,\ -0.3333,\ -0.3333,\ 0.3333,\ 0.3333,\ -0.3333)$$

It gives us the bipartition

$$(\{v_1, v_2, v_4, v_7, v_8\}, \{v_3, v_5, v_6, v_9\}),$$

as guaranteed by Proposition 5.5.

The signed Laplacian of the unbalanced graph G_2 is given by

$$\overline{L}_2 = \begin{pmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 5 & 1 & 1 & -1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 3 & 0 & -1 & -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 5 & 1 & 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 1 & 6 & -1 & 0 & 1 & -1 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 2 & -1 & 0 \\ 0 & -1 & 0 & -1 & 1 & 1 & -1 & 6 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 0 & 1 & 3 \end{pmatrix}$$

The eigenvalues of $\overline{L}_2$ are

$$0.5175,\ 1.5016,\ 1.7029,\ 2.7058,\ 3.7284,\ 4.9604,\ 5.6026,\ 7.0888,\ 8.1921.$$

The matrix $\overline{L}_2$ is indeed positive definite (since G_2 is unbalanced). Hou [14] gives bounds on the smallest eigenvalue of an unbalanced graph. The lower bound involves a measure of how unbalanced the graph is (see Theorem 3.4 in Hou [14]).

Following Kunegis et al., we can prove the following result showing that the eigenvalues and the eigenvectors of $\overline{L}$ and its unsigned counterpart $\mathcal{L}$ are strongly related. Given a symmetric signed matrix W, we define the unsigned matrix $\mathcal{W}$ such that $\mathcal{W}_{ij} = |w_{ij}|$ ($1 \leq i, j \leq m$). We let $\mathcal{L}$ be the Laplacian associated with $\mathcal{W}$. Note that

$$\mathcal{L} = \overline{D} - \mathcal{W}.$$

The following proposition is shown in Kunegis et al. [16]).

Proposition 5.7. *Let $G = (V, W)$ be a signed graph and let $\mathcal{W}$ be the unsigned matrix associated with W. If G is balanced, and x is a bipartition of V, then for any diagonalization $\overline{L} = P\Lambda P^\top$ of $\overline{L}$, where P is an orthogonal matrix of eigenvectors of $\overline{L}$, if we define the matrix $\mathcal{P}$ so that*

$$\mathcal{P}_i = x_i P_i,$$

where $\mathcal{P}_i$ is the ith row of $\mathcal{P}$ and P_i is the ith row of P, then $\mathcal{P}$ is orthogonal and

$$\mathcal{L} = \mathcal{P}\Lambda\mathcal{P}^\top$$

is a diagonalization of $\mathcal{L}$. In particular, $\overline{L}$ and $\mathcal{L}$ have the same eigenvalues with the same multiplicities.

Proof. Observe that if we let

$$X = \mathrm{diag}(x_1, \ldots, x_m),$$

then

$$\mathcal{P} = XP.$$

It follows that

$$\mathcal{P}\Lambda\mathcal{P}^\top = XP\Lambda P^\top X^\top = X\overline{L}X^\top = X\overline{L}X,$$

since X is a diagonal matrix. As a consequence, for diagonal entries, we have

$$x_i^2\overline{L}_{ii} = \overline{D}_{ii} = \mathcal{L}_{ii},$$

and for $i \neq j$, we have

$$x_i x_j \overline{L}_{ij} = \mathrm{sgn}(w_{ij})\overline{L}_{ij} = -\mathrm{sgn}(w_{ij})w_{ij} = -|w_{ij}| = -\mathcal{W}_{ij} = \mathcal{L}_{ij},$$

which proves that $\mathcal{L} = \mathcal{P}\Lambda\mathcal{P}^\top$. It remains to prove that $\mathcal{P}$ is orthogonal. Since X is a diagonal matrix whose entries are ± 1, we have $X^\top X = I$, so

$$\mathcal{P}^\top\mathcal{P} = (XP)^\top XP = P^\top X^\top XP = P^\top IP = I,$$

since P is orthogonal. Thus, $\mathcal{P}$ is indeed orthogonal. □

5.4 K-Way Clustering of Signed Graphs

Using the signed Laplacians $\overline{L}$ and $\overline{L}_{\mathrm{sym}}$, we can define the optimization problems as in Section 4.3 and solve them as in Section 4.5, except that we drop the constraint

$$X(X^\top X)^{-1}X^\top \mathbf{1} = \mathbf{1},$$

since $\mathbf{1}$ is not necessarily an eigenvector of $\overline{L}$. By Proposition A.3, the sum of the K smallest eigenvalues of $\overline{L}_{\mathrm{sym}}$ is a lower bound for $\mathrm{tr}(Y^\top\overline{L}_{\mathrm{sym}}Y)$, and the minimum of problem $(**_2)$ is achieved by any K unit eigenvectors $(u_1, \ldots, u_k)$ associated with the smallest eigenvalues

$$0 \leq \nu_1 \leq \nu_2 \leq \ldots \leq \nu_K$$

of $\overline{L}_{\mathrm{sym}}$. The difference with unsigned graphs is that ν_1 may be strictly positive. Here is the result of applying this method to various examples.

First, we apply our algorithm to find three clusters for the balanced graph G_1. The graph G_1 as outputted by the algorithm is shown in Figure 5.2 and the three clusters are shown in Figure 5.3. As desired, these clusters do not contain negative edges.

By the way, for two clusters, the algorithm finds the bipartition of G_1, as desired.

Next, we apply our algorithm to find three clusters for the unbalanced graph G_2. The graph G_2 as outputted by the algorithm is shown in Figure 5.2 and the three clusters are shown in Figure 5.3. As desired, these clusters do not contain negative edges.

The algorithm finds the same clusters, but this is probably due to the fact that G_1 and G_2 only differ by the signs of two edges.

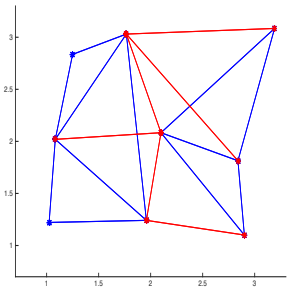

Figure 5.2: The balanced graph G_1.

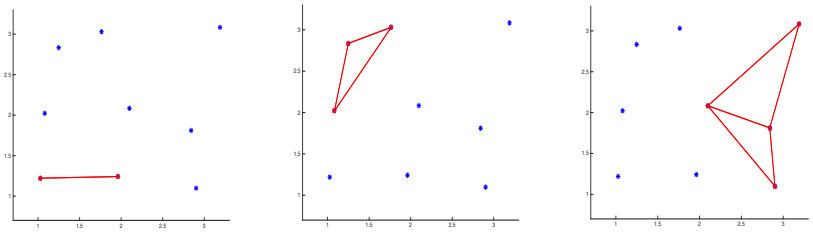

Figure 5.3: Three blocks of a normalized cut for the graph associated with G_1.

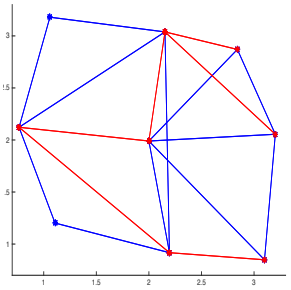

Figure 5.4: The unbalanced graph G_2.

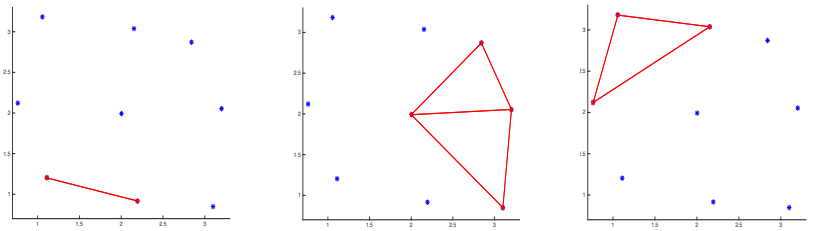

Figure 5.5: Three blocks of a normalized cut for the graph associated with G_2.

5.5 Signed Graph Drawing

Following Kunegis et al. [16], if our goal is to draw a signed graph $G = (V, W)$ with m nodes, a natural way to interpret negative weights is to assume that the endpoints v_i and v_j of an edge with a negative weight should be placed far apart, which can be achieved if instead of assigning the point $\rho(v_j) \in \mathbb{R}^n$ to v_j, we assign the point $-\rho(v_j)$. Then, if R is the $m \times n$ matrix of a graph drawing of G in $\mathbb{R}^n$, the energy function $\mathcal{E}(R)$ is redefined to be

$$\mathcal{E}(R) = \sum_{\{v_i, v_j\} \in E} |w_{ij}| \, \|\rho(v_i) - \mathrm{sgn}(w_{ij})\rho(v_j)\|^2 .$$

We obtain the following version of Proposition 3.1.

Proposition 5.8. *Let $G = (V, W)$ be a signed graph, with $|V| = m$ and with W a $m \times m$ symmetric matrix, and let R be the matrix of a graph drawing ρ of G in $\mathbb{R}^n$ (a $m \times n$ matrix). Then, we have*

$$\mathcal{E}(R) = \mathrm{tr}(R^\top \overline{L} R).$$

Proof. Since $\rho(v_i)$ is the ith row of R (and $\rho(v_j)$ is the jth row of R), if we denote the kth column of R by R^k, using Proposition 5.2, we have

$$\begin{aligned}
\mathcal{E}(R) &= \sum_{\{v_i, v_j\} \in E} |w_{ij}| \, \|\rho(v_i) - \mathrm{sgn}(w_{ij})\rho(v_j)\|^2 \\
&= \sum_{k=1}^{n} \sum_{\{v_i, v_j\} \in E} |w_{ij}| (R_{ik} - \mathrm{sgn}(w_{ij}) R_{jk})^2 \\
&= \sum_{k=1}^{n} \frac{1}{2} \sum_{i,j=1}^{m} |w_{ij}| (R_{ik} - \mathrm{sgn}(w_{ij}) R_{jk})^2 \\
&= \sum_{k=1}^{n} (R^k)^\top \overline{L} R^k = \mathrm{tr}(R^\top \overline{L} R),
\end{aligned}$$

as claimed. □

Then, as in Chapter 3, we look for a graph drawing R that minimizes $\mathcal{E}(R) = \mathrm{tr}(R^\top \overline{L} R)$ subject to $R^\top R = I$. The new ingredient is that $\overline{L}$ is positive definite iff G is not a balanced graph. Also, in the case of a signed graph, $\mathbf{1}$ does not belong to the kernel of $\overline{L}$, so we do not get a balanced graph drawing.

If G is a signed balanced graph, then $\mathrm{Ker}\, L$ is nontrivial, and if G is connected, then $\mathrm{Ker}\, L$ is spanned by a vector whose components are either $+1$ or -1. Thus, if we use the first n unit eigenvectors $(u_1, u_2, \ldots, u_n)$ associated with the n smallest eigenvalues $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ of $\overline{L}$, we obtain a drawing for which the nodes are partitionned into two sets living in two hyperplanes corresponding to the value of their first coordinate. Let us call such a drawing a *bipartite drawing*. However, if G is connected, the vector u_2 does not

belong to $\operatorname{Ker} \overline{L}$, so if $m \geq 3$, it must have at least three coordinates with distinct absolute values, and using $(u_2, \ldots, u_{n+1})$ we obtain a nonbipartite graph. Then, the following version of Theorem 3.2 is easily shown.

Theorem 5.9. *Let $G = (V, W)$ be a signed graph with $|V| = m \geq 3$, assume that G has some negative edge and is connected, and let $\overline{L} = \overline{D} - W$ be the signed Laplacian of G.*

(1) If G is not balanced and if the eigenvalues of L are $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_m$, then the minimal energy of any orthogonal graph drawing of G in $\mathbb{R}^n$ is equal to $\lambda_1 + \cdots + \lambda_n$ The $m \times n$ matrix R consisting of any unit eigenvectors $u_1, \ldots, u_n$ associated with $\lambda_1 \leq \ldots \leq \lambda_n$ yields an orthogonal graph drawing of minimal energy.

(2) If G is balanced and if the eigenvalues of L are $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_m$, then the minimal energy of any orthogonal nonbipartite graph drawing of G in $\mathbb{R}^n$ is equal to $\lambda_2 + \cdots + \lambda_{n+1}$ (in particular, this implies that $n < m$). The $m \times n$ matrix R consisting of any unit eigenvectors $u_2, \ldots, u_{n+1}$ associated with $\lambda_2 \leq \ldots \leq \lambda_{n+1}$ yields an orthogonal nonbipartite graph drawing of minimal energy.

(3) If G is balanced, for $n = 2$, a graph drawing of G as a bipartite graph (with positive edges only withing the two blocks of vertices) is obtained from the $m \times 2$ matrix consisting of any two unit eigenvectors u_1 and u_2 associated with 0 and λ_2.

In all cases, the graph drawing R satisfies the condition $R^\top R = I$ (it is an orthogonal graph drawing).

Our first example is the signed graph $G4$ defined by the weight matrix given by the following `Matlab` program:

```
nn = 6; G3 = diag(ones(1,nn),1); G3 = G3 + G3';
G3(1,nn+1) = 1; G3(nn+1,1) = 1; G4 = -G3;
```

All edges of this graph are negative. The graph obtained by using $G3$ is shown on the left and the graph obtained by using the signed Laplacian of $G4$ is shown on the right in Figure 5.6.

The second example is the signed graph $G5$ obtained from $G3$ by making a single edge negative:

```
G5 = G3; G5(1,2) = -1; G5(2,1) = -1;
```

The graph obtained by using $G3$ is shown on the left and the graph obtained by using the signed Laplacian of $G5$ is shown on the right in Figure 5.7. Positive edges are shown in blue and negative edges are shown in red.

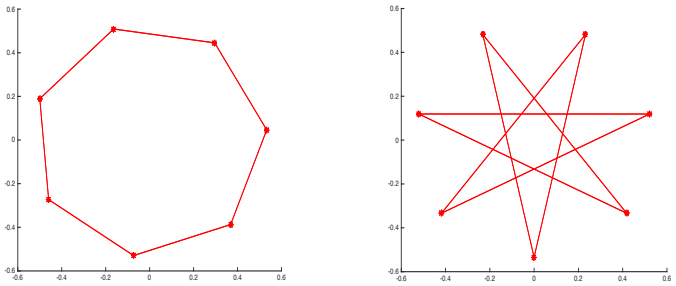

Figure 5.6: The signed graph $G4$.

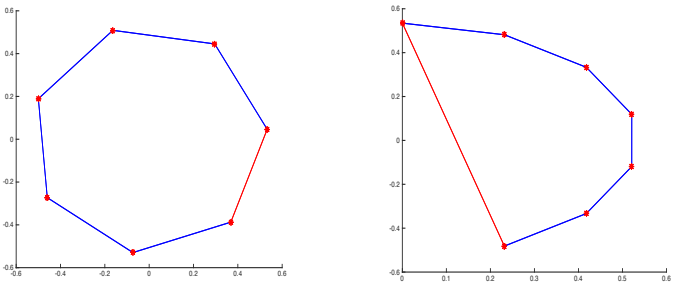

Figure 5.7: The signed graph $G5$.

The third example is the signed graph $G6$ defined by the weight matrix given by the following `Matlab` program:

```
nn = 24; G6 = diag(ones(1,nn),1); G6 = G6 + G6';
G6(1,nn+1) = 1; G6(nn+1,1) = 1;
G6(1,2) = -1; G6(2,1) = -1; G6(6,7) = -1; G6(7,6) = -1;
G6(11,12) = -1; G6(12,11) = -1; G6(16,17) = -1; G6(17,16) = -1;
G6(21,22) = -1; G6(22,21) = -1;
```

The graph obtained by using absolute values in $G6$ is shown on the left and the graph obtained by using the signed Laplacian of $G6$ is shown on the right in Figure 5.8.

The fourth example is the signed graph $G7$ defined by the weight matrix given by the following `Matlab` program:

```
nn = 26; G7 = diag(ones(1,nn),1); G7 = G7 + G7';
G7(1,nn+1) = 1; G7(nn+1,1) = 1;
G7(1,2) = -1; G7(2,1) = -1; G7(10,11) = -1; G7(11,10) = -1;
G7(19,20) = -1; G7(20,19) = -1;
```

The graph obtained by using absolute values in $G7$ is shown on the left and the graph obtained by using the signed Laplacian of $G7$ is shown on the right in Figure 5.9.

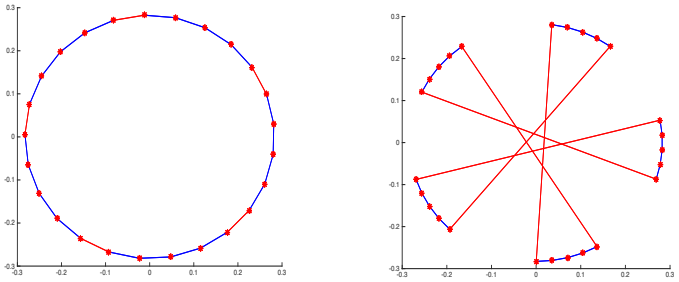

Figure 5.8: The signed graph $G6$.

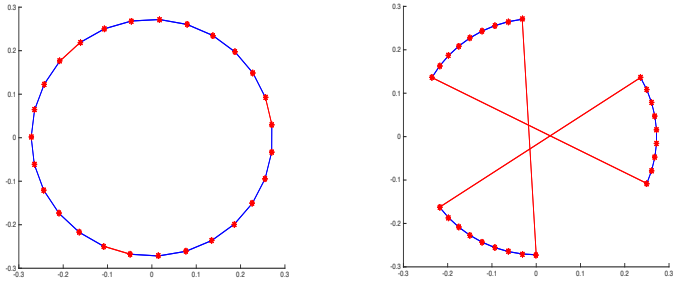

Figure 5.9: The signed graph $G7$.

These graphs are all unbalanced. As predicted, nodes linked by negative edges are far from each other.

Our last example is the balanced graph $G1$ from Figure 5.1. The graph obtained by using absolute values in $G1$ is shown on the left and the bipartite graph obtained by using the signed Laplacian of $G1$ is shown on the right in Figure 5.10.

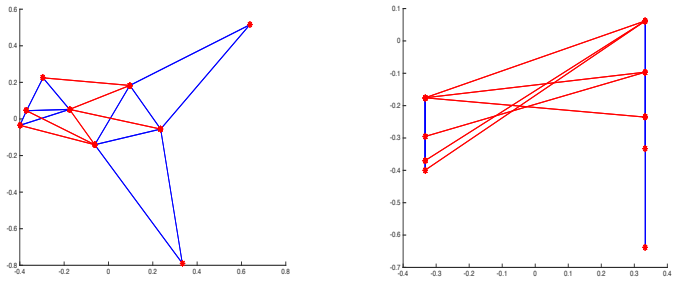

Figure 5.10: The balanced graph $G1$.

Chapter 6

Graph Clustering Using Ratio Cuts

In this short chapter, we consider the alternative to normalized cut, called ratio cut, and show that the methods of Chapters 4 and 5 can be trivially adapted to solve the clustering problem using ratio cuts. All that needs to be done is to replace the normalized Laplacian L_{sym} by the unormalized Laplacian L, and omit the step of considering Problem $(**_2)$. In particular, there is no need to multiply the continuous solution Y by $D^{-1/2}$. The idea of ratio cut is to replace the volume $\mathrm{vol}(A_j)$ of each block A_j of the partition by its size, $|A_j|$ (the number of nodes in A_j). First, we deal with unsigned graphs, the case where the entries in the symmetric weight matrix W are nonnegative.

Definition 6.1. The *ratio cut* $\mathrm{Rcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ is defined as

$$\mathrm{Rcut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{|A_j|}.$$

As in Section 4.3, given a partition of V into K clusters $(A_1, \ldots, A_K)$, if we represent the jth block of this partition by a vector X^j such that

$$X_i^j = \begin{cases} a_j & \text{if } v_i \in A_j \\ 0 & \text{if } v_i \notin A_j, \end{cases}$$

for some $a_j \neq 0$, then

$$\begin{aligned} (X^j)^\top L X^j &= a_j^2(\mathrm{cut}(A_j, \overline{A_j}) \\ (X^j)^\top X^j &= a_j^2 |A_j|. \end{aligned}$$

Consequently, we have

$$\mathrm{Rcut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{|A_j|} = \sum_{i=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top X^j}.$$

On the other hand, the normalized cut is given by

$$\mathrm{Ncut}(A_1, \ldots, A_K) = \sum_{i=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A}_j)}{\mathrm{vol}(A_j)} = \sum_{i=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top D X^j}.$$

Therefore, ratio cut is the special case of normalized cut where $D = I$. If we let

$$\mathcal{X} = \Big\{[X^1 \ \ldots \ X^K] \mid X^j = a_j(x_1^j, \ldots, x_N^j),\ x_i^j \in \{1, 0\}, a_j \in \mathbb{R},\ X^j \neq 0\Big\}$$

(note that the condition $X^j \neq 0$ implies that $a_j \neq 0$), then the set of matrices representing partitions of V into K blocks is

$$\mathcal{K} = \Big\{X = [X^1 \ \cdots \ X^K] \quad | \quad X \in \mathcal{X}, \\ (X^i)^\top X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j\Big\}.$$

Here is our first formulation of K-way clustering of a graph using ratio cuts, called problem PRC1 :

K-way Clustering of a graph using Ratio Cut, Version 1:
Problem PRC1

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{j=1}^{K} \frac{(X^j)^\top L X^j}{(X^j)^\top X^j} \\ \text{subject to} & (X^i)^\top X^j = 0, \quad 1 \leq i, j \leq K,\ i \neq j, \\ & X \in \mathcal{X}. \end{array}$$

The solutions that we are seeking are K-tuples $(\mathbb{P}(X^1), \ldots, \mathbb{P}(X^K))$ of points in $\mathbb{RP}^{N-1}$ determined by their homogeneous coordinates $X^1, \ldots, X^K$. As in Chapter 4, chasing denominators and introducing a trace, we obtain the following formulation of our minimization problem:

K-way Clustering of a graph using Ratio Cut, Version 2:
Problem PRC2

$$\begin{array}{ll} \text{minimize} & \mathrm{tr}(X^\top L X) \\ \text{subject to} & X^\top X = I, \\ & X \in \mathcal{X}. \end{array}$$

The natural relaxation of problem PRC2 is to drop the condition that $X \in \mathcal{X}$, and we obtain the

Problem $(R*_2)$

minimize	$\mathrm{tr}(X^\top LX)$
subject to	$X^\top X = I.$

This time, since the normalization condition is $X^\top X = I$, we can use the eigenvalues and the eigenvectors of L, and by Proposition A.2, the minimum is achieved by any K unit eigenvectors $(u_1, \ldots, u_K)$ associated with the smallest K eigenvalues

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_K$$

of L. The matrix $Z = Y = [u_1, \ldots, u_K]$ yields a minimum of our relaxed problem $(R*_2)$. The rest of the algorithm is as before; we try to find $Q = R\Lambda$ with $R \in \mathbf{O}(K)$, Λ diagonal invertible, and $X \in \mathcal{X}$ such that $\|X - ZQ\|$ is minimum.

In the case of signed graphs, we define the *signed ratio cut* $\mathrm{sRcut}(A_1, \ldots, A_K)$ of the partition $(A_1, \ldots, A_K)$ as

$$\mathrm{sRcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{\mathrm{cut}(A_j, \overline{A_j})}{|A_j|} + 2\sum_{j=1}^{K} \frac{\mathrm{links}^-(A_j, A_j)}{|A_j|}.$$

Since we still have

$$(X^j)^\top \overline{L} X^j = a_j^2(\mathrm{cut}(A_j, \overline{A_j}) + 2\mathrm{links}^-(A_j, A_j)),$$

we obtain

$$\mathrm{sRcut}(A_1, \ldots, A_K) = \sum_{j=1}^{K} \frac{(X^j)^\top \overline{L} X^j}{(X^j)^\top X^j}.$$

Therefore, this is similar to the case of unsigned graphs, with L replaced with $\overline{L}$. The same algorithm applies, but as in Chapter 5, the signed Laplacian $\overline{L}$ is positive definite iff G is unbalanced. Modifying the computer program implementing normalized cuts to deal with ratio cuts is trivial (use $\overline{L}$ instead of $\overline{L}_{\mathrm{sym}}$ and don't multiply Y by $\overline{D}^{-1/2}$). Generally, normalized cut seems to yield "better clusters," but this is not a very satisfactory statement since we haven't defined precisely in which sense a clustering is better than another. We leave this point as further research.

Appendix A

Rayleigh Ratios and the Courant-Fischer Theorem

The most important property of symmetric matrices is that they have real eigenvalues and that they can be diagonalized with respect to an orthogonal matrix. Thus, if A is an $n \times n$ symmetric matrix, then it has n real eigenvalues $\lambda_1, \ldots, \lambda_n$ (not necessarily distinct), and there is an orthonormal basis of eigenvectors $(u_1, \ldots, u_n)$ (for a proof, see Gallier [8]). Another fact that is used frequently in optimization problem is that the eigenvalues of a symmetric matrix are characterized in terms of what is known as the *Rayleigh ratio*, defined by

$$R(A)(x) = \frac{x^\top Ax}{x^\top x}, \quad x \in \mathbb{R}^n, x \neq 0.$$

The following proposition is often used to prove the correctness of various optimization or approximation problems (for example PCA).

Proposition A.1. *(Rayleigh–Ritz) If A is a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and if $(u_1, \ldots, u_n)$ is any orthonormal basis of eigenvectors of A, where u_i is a unit eigenvector associated with λ_i, then*

$$\max_{x \neq 0} \frac{x^\top Ax}{x^\top x} = \lambda_n$$

(with the maximum attained for $x = u_n$), and

$$\max_{x \neq 0, x \in \{u_{n-k+1}, \ldots, u_n\}^\perp} \frac{x^\top Ax}{x^\top x} = \lambda_{n-k}$$

(with the maximum attained for $x = u_{n-k}$), where $1 \leq k \leq n-1$. Equivalently, if V_k is the subspace spanned by $(u_1, \ldots, u_k)$, then

$$\lambda_k = \max_{x \neq 0, x \in V_k} \frac{x^\top Ax}{x^\top x}, \quad k = 1, \ldots, n.$$

Proof. First, observe that

$$\max_{x\neq 0}\frac{x^\top Ax}{x^\top x} = \max_x\{x^\top Ax \mid x^\top x = 1\},$$

and similarly,

$$\max_{x\neq 0, x\in\{u_{n-k+1},\ldots,u_n\}^\perp}\frac{x^\top Ax}{x^\top x} = \max_x\left\{x^\top Ax \mid (x\in\{u_{n-k+1},\ldots,u_n\}^\perp)\wedge(x^\top x = 1)\right\}.$$

Since A is a symmetric matrix, its eigenvalues are real and it can be diagonalized with respect to an orthonormal basis of eigenvectors, so let $(u_1,\ldots,u_n)$ be such a basis. If we write

$$x = \sum_{i=1}^n x_i u_i,$$

a simple computation shows that

$$x^\top Ax = \sum_{i=1}^n \lambda_i x_i^2.$$

If $x^\top x = 1$, then $\sum_{i=1}^n x_i^2 = 1$, and since we assumed that $\lambda_1\leq\lambda_2\leq\cdots\leq\lambda_n$, we get

$$x^\top Ax = \sum_{i=1}^n \lambda_i x_i^2 \leq \lambda_n\left(\sum_{i=1}^n x_i^2\right) = \lambda_n.$$

Thus,

$$\max_x\left\{x^\top Ax \mid x^\top x = 1\right\}\leq\lambda_n,$$

and since this maximum is achieved for $e_n = (0,0,\ldots,1)$, we conclude that

$$\max_x\left\{x^\top Ax \mid x^\top x = 1\right\} = \lambda_n.$$

Next, observe that $x\in\{u_{n-k+1},\ldots,u_n\}^\perp$ and $x^\top x = 1$ iff $x_{n-k+1} = \cdots = x_n = 0$ and $\sum_{i=1}^{n-k} x_i^2 = 1$. Consequently, for such an x, we have

$$x^\top Ax = \sum_{i=1}^{n-k} \lambda_i x_i^2 \leq \lambda_{n-k}\left(\sum_{i=k+1}^{n} x_i^2\right) = \lambda_{n-k}.$$

Thus,

$$\max_x\left\{x^\top Ax \mid (x\in\{u_{n-k+1},\ldots,u_n\}^\perp)\wedge(x^\top x = 1)\right\}\leq\lambda_{n-k},$$

and since this maximum is achieved for $e_{n-k} = (0,\ldots,0,1,0,\ldots,0)$ with a 1 in position $n-k$, we conclude that

$$\max_x\left\{x^\top Ax \mid (x\in\{u_{n-k+1},\ldots,u_n\}^\perp)\wedge(x^\top x = 1)\right\} = \lambda_{n-k},$$

as claimed. □

For our purposes, we also need the version of Proposition A.1 applying to min instead of max, whose proof is obtained by a trivial modification of the proof of Proposition A.1.

Proposition A.2. *(Rayleigh–Ritz) If A is a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and if $(u_1, \ldots, u_n)$ is any orthonormal basis of eigenvectors of A, where u_i is a unit eigenvector associated with λ_i, then*

$$\min_{x \neq 0} \frac{x^\top A x}{x^\top x} = \lambda_1$$

(with the minimum attained for $x = u_1$), and

$$\min_{x \neq 0, x \in \{u_1, \ldots, u_{i-1}\}^\perp} \frac{x^\top A x}{x^\top x} = \lambda_i$$

(with the minimum attained for $x = u_i$), where $2 \leq i \leq n$. Equivalently, if $W_k = V_{k-1}^\perp$ denotes the subspace spanned by $(u_k, \ldots, u_n)$ (with $V_0 = (0)$), then

$$\lambda_k = \min_{x \neq 0, x \in W_k} \frac{x^\top A x}{x^\top x} = \min_{x \neq 0, x \in V_{k-1}^\perp} \frac{x^\top A x}{x^\top x}, \quad k = 1, \ldots, n.$$

Propositions A.1 and A.2 together are known as the *Rayleigh–Ritz theorem*.

As an application of Propositions A.1 and A.2, we give a proof of a proposition which is the key to the proof of Theorem 3.2. First, we need a definition. Given an $n \times n$ symmetric matrix A and an $m \times m$ symmetric B, with $m \leq n$, if $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of A and $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_m$ are the eigenvalues of B, then we say that the eigenvalues of B *interlace* the eigenvalues of A if

$$\lambda_i \leq \mu_i \leq \lambda_{n-m+i}, \quad i = 1, \ldots, m.$$

The following proposition is known as the *Poincaré separation theorem*; see Horn and Johnson [13], Section 4.3, Corollary 4.3.16.

Proposition A.3. *Let A be an $n \times n$ symmetric matrix, R be an $n \times m$ matrix such that $R^\top R = I$ (with $m \leq n$), and let $B = R^\top A R$ (an $m \times m$ matrix). The following properties hold:*

(a) The eigenvalues of B interlace the eigenvalues of A.

(b) If $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of A and $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_m$ are the eigenvalues of B, and if $\lambda_i = \mu_i$, then there is an eigenvector v of B with eigenvalue μ_i such that Rv is an eigenvector of A with eigenvalue λ_i.

Proof. (a) Let $(u_1, \ldots, u_n)$ be an orthonormal basis of eigenvectors for A, and let $(v_1, \ldots, v_m)$ be an orthonormal basis of eigenvectors for B. Let U_j be the subspace spanned by $(u_1, \ldots, u_j)$ and let V_j be the subspace spanned by $(v_1, \ldots, v_j)$. For any i, the subpace V_i has dimension i and the subspace $R^\top U_{i-1}$ has dimension at most $i-1$. Therefore, there is some nonzero vector $v \in V_i \cap (R^\top U_{i-1})^\perp$, and since

$$v^\top R^\top u_j = (Rv)^\top u_j = 0, \quad j = 1, \ldots, i-1,$$

we have $Rv \in (U_{i-1})^\perp$. By Proposition A.2 and using the fact that $R^\top R = I$, we have

$$\lambda_i \leq \frac{(Rv)^\top ARv}{(Rv)^\top Rv} = \frac{v^\top Bv}{v^\top v}.$$

On the other hand, by Proposition A.1,

$$\mu_i = \max_{x \neq 0, x \in \{v_{i+1}, \ldots, v_n\}^\perp} \frac{x^\top Bx}{x^\top x} = \max_{x \neq 0, x \in \{v_1, \ldots, v_i\}} \frac{x^\top Bx}{x^\top x},$$

so

$$\frac{w^\top Bw}{w^\top w} \leq \mu_i \quad \text{for all } w \in V_i,$$

and since $v \in V_i$, we have

$$\lambda_i \leq \frac{v^\top Bv}{v^\top v} \leq \mu_i, \quad i = 1, \ldots, m.$$

We can apply the same argument to the symmetric matrices $-A$ and $-B$, to conclude that

$$-\lambda_{n-m+i} \leq -\mu_i,$$

that is,

$$\mu_i \leq \lambda_{n-m+i}, \quad i = 1, \ldots, m.$$

Therefore,

$$\lambda_i \leq \mu_i \leq \lambda_{n-m+i}, \quad i = 1, \ldots, m,$$

as desired.

(b) If $\lambda_i = \mu_i$, then

$$\lambda_i = \frac{(Rv)^\top ARv}{(Rv)^\top Rv} = \frac{v^\top Bv}{v^\top v} = \mu_i,$$

so v must be an eigenvector for B and Rv must be an eigenvector for A, both for the eigenvalue $\lambda_i = \mu_i$. □

Observe that Proposition A.3 implies that

$$\lambda_1 + \cdots + \lambda_m \leq \operatorname{tr}(R^\top AR) \leq \lambda_{n-m+1} + \cdots + \lambda_n.$$

The left inequality is used to prove Theorem 3.2.

For the sake of completeness, we also prove the Courant–Fischer characterization of the eigenvalues of a symmetric matrix.

Theorem A.4. *(Courant–Fischer) Let A be a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and let $(u_1, \ldots, u_n)$ be any orthonormal basis of eigenvectors of A, where u_i is a unit eigenvector associated with λ_i. If $\mathcal{V}_k$ denotes the set of subspaces of $\mathbb{R}^n$ of dimension k, then*

$$\lambda_k = \max_{W \in \mathcal{V}_{n-k+1}} \min_{x \in W, x \neq 0} \frac{x^\top A x}{x^\top x}$$
$$\lambda_k = \min_{W \in \mathcal{V}_k} \max_{x \in W, x \neq 0} \frac{x^\top A x}{x^\top x}.$$

Proof. Let us consider the second equality, the proof of the first equality being similar. Observe that the space V_k spanned by $(u_1, \ldots, u_k)$ has dimension k, and by Proposition A.1, we have

$$\lambda_k = \max_{x \neq 0, x \in V_k} \frac{x^\top A x}{x^\top x} \geq \min_{W \in \mathcal{V}_k} \max_{x \in W, x \neq 0} \frac{x^\top A x}{x^\top x}.$$

Therefore, we need to prove the reverse inequality; that is, we have to show that

$$\lambda_k \leq \max_{x \neq 0, x \in W} \frac{x^\top A x}{x^\top x}, \quad \text{for all} \quad W \in \mathcal{V}_k.$$

Now, for any $W \in \mathcal{V}_k$, if we can prove that $W \cap V_{k-1}^\perp \neq (0)$, then for any nonzero $v \in W \cap V_{k-1}^\perp$, by Proposition A.2 , we have

$$\lambda_k = \min_{x \neq 0, x \in V_{k-1}^\perp} \frac{x^\top A x}{x^\top x} \leq \frac{v^\top A v}{v^\top v} \leq \max_{x \in W, x \neq 0} \frac{x^\top A x}{x^\top x}.$$

It remains to prove that $\dim(W \cap V_{k-1}^\perp) \geq 1$. However, $\dim(V_{k-1}) = k - 1$, so $\dim(V_{k-1}^\perp) = n - k + 1$, and by hypothesis $\dim(W) = k$. By the Grassmann relation,

$$\dim(W) + \dim(V_{k-1}^\perp) = \dim(W \cap V_{k-1}^\perp) + \dim(W + V_{k-1}^\perp),$$

and since $\dim(W + V_{k-1}^\perp) \leq \dim(\mathbb{R}^n) = n$, we get

$$k + n - k + 1 \leq \dim(W \cap V_{k-1}^\perp) + n;$$

that is, $1 \leq \dim(W \cap V_{k-1}^\perp)$, as claimed. □

Appendix B

Riemannian Metrics on Quotient Manifolds

In order to define a metric on the projective space $\mathbb{RP}^n$, we need to review a few notions of differential geometry. First, we need to define the quotient M/G of a manifold by a group acting on M. This section relies heavily on Gallot, Hulin, Lafontaine [9] and Lee [17], which contain thorough expositions and should be consulted for details.

Definition B.1. Recall that an *action* of a group G (with identity element 1) on a set X is a map $\gamma\colon G \times X \to X$ satisfying the following properties:

(1) $\gamma(1, x) = x$, for all $x \in X$.

(2) $\gamma(g_1, \gamma(g_2, x)) = \gamma(g_1 g_2, x)$, for all $g_1, g_2 \in G$, and all $x \in X$.

We usually abbreviate $\gamma(g, x)$ by $g \cdot x$.

If X is a topological space and G is a topological group, we say that the action is *continuous* iff the map γ is continuous. In this case, for every $g \in G$, the map $x \mapsto g \cdot x$ is a homeomorphism. If X is a smooth manifold and G is a Lie group, we say that the action is *smooth* iff the map γ is smooth. In this case, for every $g \in G$, the map $x \mapsto g \cdot x$ is a diffeomorphism.

Remark: To be more precise, what we have defined in Definition B.1 is a *left action* of the group G on the set X. There is also a notion of a *right action*, but we won't need it.

The *quotient of X by G*, denoted X/G, is the set of orbits of G; that is, the set of equivalences classes of the equivalence relation $\simeq$ defined such that, for any $x, y \in X$,

$$x \simeq y \quad \text{iff} \quad (\exists g \in G)(y = g \cdot x).$$

The *orbit* of $x \in X$ (the equivalence class of x) is the set

$$O(x) = \{g \cdot x \mid g \in G\},$$

also denoted by $G \cdot x$. If X is a topological space, we give X/G the quotient topology.

For any subset V of X and for any $g \in G$, we denote by gV the set

$$gV = \{g \cdot x \mid x \in V\}.$$

One problem is that even if X is Hausdorff, X/G may not be. Thus, we need to find conditions to ensure that X/G is Hausdorff.

By a *discrete group*, we mean a group equipped with the discrete topology (every subset is open). In other words, we don't care about the topology of G! The following conditions prove to be useful.

Definition B.2. Let $\cdot : G \times X \to X$ be the action of a group G on a set X. We say that G acts *freely* (or that the action is *free*) iff for all $g \in G$ and all $x \in X$, if $g \neq 1$ then $g \cdot x \neq x$.

If X is a locally compact space and G is a discrete group acting continuously on X, we say that G acts *properly* (or that the action is *proper*) iff

(i) For every $x \in X$, there is some open subset V with $x \in V$ such that $gV \cap V \neq \emptyset$ for only finitely many $g \in G$.

(ii) For all $x, y \in X$, if $y \notin G \cdot x$ (y is not in the orbit of x), then there exist some open sets V, W with $x \in V$ and $y \in W$ such that $gV \cap W = 0$ for all $g \in G$.

The following proposition gives necessary and sufficient conditions for a discrete group to act freely and properly often found in the literature (for instance, O'Neill [18], Berger and Gostiaux [3], and do Carmo [6], but beware that in this last reference Hausdorff separation is not required!).

Proposition B.1. *If X is a locally compact space and G is a discrete group, then a smooth action of G on M is free and proper iff the following conditions hold:*

(i) For every $x \in X$, there is some open subset V with $x \in V$ such that $gV \cap V = \emptyset$ for all $g \in G$ such that $g \neq 1$.

(ii) For all $x, y \in X$, if $y \notin G \cdot x$ (y is not in the orbit of x), then there exist some open sets V, W with $x \in V$ and $y \in W$ such that $gV \cap W = 0$ for all $g \in G$.

Proof. Condition (i) of Proposition B.1 implies condition (i) of Definition B.2, and condition (ii) is the same in Proposition B.1 and Definition B.2. If (i) holds, then the action must be free since if $g \cdot x = x$, then $gV \cap V \neq \emptyset$, which implies that $g = 1$.

Conversely, we just have to prove that the conditions of Definition B.2 imply condition (i) of Proposition B.1. By (i) of Definition B.2, there is some open subset U containing x and a finite number of elements of G, say $g_1, \ldots, g_m$, with $g_i \neq 1$, such that

$$g_i U \cap U \neq \emptyset, \quad i = 1, \ldots, m.$$

Since our action is free and $g_i \neq 1$, we have $g_i \cdot x \neq x$, so by Hausdorff separation, there exist some open subsets W_i, W_i', with $x \in W_i$ and $g_i \cdot x \in W_i'$, such that $W_i \cap W_i' = \emptyset$, $i = 1, \ldots, m$. Then, if we let

$$V = W \cap \left(\bigcap_{i=1}^{m} (W_i \cap g_i^{-1} W_i') \right),$$

we see that $V \cap g_i V = \emptyset$, and since $V \subseteq W$, we also have $V \cap gV = \emptyset$ for all other $g \in G$. $\square$

Remark: The action of a discrete group satisfying the properties of Proposition B.1 is often called "properly discontinuous." However, as pointed out by Lee ([17], just before Proposition 9.18), this term is self-contradictory since such actions are smooth, and thus continuous!

We also need covering maps.

Definition B.3. Let X and Y be two topological spaces. A map $\pi \colon X \to Y$ is a *covering map* iff the following conditions hold:

(1) The map π is continuous and surjective.

(2) For every $y \in Y$, there is some open subset $W \subseteq Y$ with $y \in W$, such that

$$\pi^{-1}(W) = \bigcup_{i \in I} U_i,$$

where the $U_i \subseteq X$ are pairwise disjoint open subsets such that the restriction of π to U_i is a homeomorphism for every $i \in I$.

If X and Y are smooth manifolds, we assume that π is smooth and that the restriction of π to each U_i is a diffeomorphism.

Then, we have the following useful result.

Theorem B.2. *Let M be a smooth manifold and let G be discrete group acting smoothly, freely and properly on M. Then there is a unique structure of smooth manifold on M/G such that the projection map $\pi \colon M \to M/G$ is a covering map.*

For a proof, see Gallot, Hulin, Lafontaine [9] (Theorem 1.88) or Lee [17] (Theorem 9.19).

Real projective spaces are illustrations of Theorem B.2. Indeed, if M is the unit n-sphere $S^n \subseteq \mathbb{R}^{n+1}$ and $G = \{I, -I\}$, where $-I$ is the antipodal map, then the conditions of Proposition B.1 are easily checked (since S^n is compact), and consequently the quotient

$$\mathbb{RP}^n = S^n/G$$

is a smooth manifold and the projection map $\pi \colon S^n \to \mathbb{RP}^n$ is a covering map. The fiber $\pi^{-1}([x])$ of every point $[x] \in \mathbb{RP}^n$ consists of two antipodal points: $x, -x \in S^n$.

The next step is see how a Riemannian metric on M induces a Riemannian metric on the quotient manifold M/G.

Definition B.4. Given any two Riemmanian manifolds (M, g) and (N, h) a smooth map $f\colon M \to N$ is a *local isometry* iff for all $p \in M$, the tangent map $df_p\colon T_pM \to T_{f(p)}N$ is an orthogonal transformation of the Euclidean spaces (T_pM, g_p) and $(T_{f(p)}N, h_{f(p)}))$. Furthermore, if f is a diffeomorphism, we say that f is an *isometry*.

The Riemannian version of a covering map is the following:

Definition B.5. Let (M, g) and (N, h) be two Riemannian manifolds. A map $\pi\colon M \to N$ is a *Riemannian covering map* iff the following conditions hold:

(1) The map π is a smooth covering.

(2) The map π is a local isometry.

The following theorem is the Riemannian version of Theorem B.2.

Theorem B.3. *Let (M, h) be a Riemannian manifold and let G be discrete group acting smoothly, freely and properly on M, and such that the map $x \mapsto \sigma \cdot x$ is an isometry for all $\sigma \in G$. Then there is a unique structure of Riemannian manifold on $N = M/G$ such that the projection map $\pi\colon M \to M/G$ is a Riemannian covering map.*

Proof sketch. For a complete proof see Gallot, Hulin, Lafontaine [9] (Proposition 2.20). To define a Riemannian metric g on $N = M/G$ we need to define an inner product g_p on the tangent space T_pN for every $p \in N$. Pick any $q_1 \in \pi^{-1}(p)$ in the fibre of p. Because π is a Riemannian covering map, it is a local diffeomorphism, and thus $d\pi_{q_1}\colon T_{q_1}M \to T_pM$ is an isometry. Then, given any two tangent vectors $u, v \in T_pN$, we define their inner product $g_p(u, v)$ by

$$g_p(u, v) = h_{q_1}(d\pi_{q_1}^{-1}(u), d\pi_{q_1}^{-1}(v)).$$

Now, we need to show that g_p does not depend on the choice of $q_1 \in \pi^{-1}(p)$. So, let $q_2 \in \pi^{-1}(p)$ be any other point in the fibre of p. By definition of $N = M/G$, we have $q_2 = g \cdot q_1$ for some $g \in G$, and we know that the map $f\colon q \mapsto g \cdot q$ is an isometry of M. Now, since $\pi = \pi \circ f$ we have

$$d\pi_{q_1} = d\pi_{q_2} \circ df_{q_1},$$

and since $d\pi_{q_1}\colon T_{q_1}M \to T_pM$ and $d\pi_{q_2}\colon T_{q_2}M \to T_pM$ are isometries, we get

$$d\pi_{q_2}^{-1} = df_{q_1} \circ d\pi_{q_1}^{-1}.$$

But $df_{q_1}\colon T_{q_1}M \to T_{q_2}M$ is also an isometry, so

$$h_{q_2}(d\pi_{q_2}^{-1}(u), d\pi_{q_2}^{-1}(v)) = h_{q_2}(df_{q_1}(d\pi_{q_1}^{-1}(u)), df_{q_1}(d\pi_{q_2}^{-1}(v))) = h_{q_1}(d\pi_{q_1}^{-1}(u), d\pi_{q_1}^{-1}(v)).$$

Therefore, the inner product g_p is well defined on T_pN. □

Theorem B.3 implies that every Riemannian metric g on the sphere S^n induces a Riemannian metric $\widehat{g}$ on the projective space $\mathbb{RP}^n$, in such a way that the projection $\pi\colon S^n \to \mathbb{RP}^n$ is a Riemannian covering. In particular, if U is an open hemisphere obtained by removing its boundary S^{n-1} from a closed hemisphere, then π is an isometry between U and its image $\mathbb{RP}^n - \pi(S^{n-1}) \approx \mathbb{RP}^n - \mathbb{RP}^{n-1}$.

We also observe that for any two points $p = [x]$ and $q = [y]$ in $\mathbb{RP}^n$, where $x, y \in S^n$, if $x \cdot y = \cos\theta$, with $0 \leq \theta \leq \pi$, then there are two possibilities:

1. $x \cdot y \geq 0$, which means that $0 \leq \theta \leq \pi/2$, or

2. $x \cdot y < 0$, which means that $\pi/2 < \theta \leq \pi$.

In the second case, since $[-y] = [y]$ and $x \cdot (-y) = -x \cdot y$, we can replace the representative y of q by $-y$, and we have $x \cdot (-y) = \cos(\pi - \theta)$, with $0 \leq \pi - \theta < \pi/2$. Therefore, in all cases, for any two points $p, q \in \mathbb{RP}^n$, we can find an open hemisphere U such that $p = [x], q = [y]$, $x, y \in U$, and $x \cdot y \geq 0$; that is, the angle $\theta \geq 0$ between x and y is at most $\pi/2$. This fact together with the following simple proposition will allow us to figure out the distance (in the sense of Riemannian geometry) between two points in $\mathbb{RP}^n$.

Proposition B.4. *Let $\pi\colon M \to N$ be a Riemannian covering map between two Riemannian manifolds (M, g) and (N, h). Then, the geodesics of (N, h) are the projections of geodesics in (M, g) (i.e., curves $\pi \circ \gamma$ in (N, h), where γ is a geodesic in (M, g)), and the geodesics of (M, g) are the liftings of geodesics in (N, h) (i.e., curves γ of (M, g), such that $\pi \circ \gamma$ is a geodesic in (N, h)).*

The proof of Proposition B.4 can be found in Gallot, Hulin, Lafontaine [9] (Proposition 2.81).

Now, if (M, g) is a connected Riemannian manifold, recall that we define the distance $d(p, q)$ between two points $p, q \in M$ as

$$d(p, q) = \inf\{L(\gamma) \mid \gamma\colon [0, 1] \to M\},$$

where γ is any piecewise C^1-curve from p to q, and

$$L(\gamma) = \int_0^1 \sqrt{g(\gamma'(t), \gamma'(t))}\, dt$$

is the length of γ. It is well known that d is a metric on M. The Hopf-Rinow Theorem (see Gallot, Hulin, Lafontaine [9], Theorem 2.103) says among other things that (M, g) is geodesically complete (which means that every geodesics γ of M can be extended to a geodesic $\widetilde{\gamma}$ defined on all of $\mathbb{R}$) iff any two points of M can be joined by a minimal geodesic iff (M, d) is a complete metric space. Therefore, in a complete (connected) manifold

$$d(p, q) = \inf\{L(\gamma) \mid \gamma\colon [0, 1] \to M \quad \text{is a geodesic}\}.$$

In particular, compact manifolds are complete, so the distance between two points is the infimum of the length of minimal geodesics joining these points.

Applying this to $\mathbb{RP}^n$ and the canonical Euclidean metric induced by $\mathbb{R}^{n+1}$, since geodesics of S^n are great circles, by the discussion above, for any two points $p = [x]$ and $q = [y]$ in $\mathbb{RP}^n$, with $x, y \in S^n$, the distance between them is given by

$$d(p,q) = d([x],[y]) = \begin{cases} \cos^{-1}(x \cdot y) & \text{if } x \cdot y \geq 0 \\ \cos^{-1}(-x \cdot y) & \text{if } x \cdot y < 0. \end{cases}$$

Here $\cos^{-1}(z) = \arccos(z)$ is the unique angle $\theta \in [0, \pi]$ such that $\cos(\theta) = z$. Equivalently,

$$d([x],[y]) = \cos^{-1}(|x \cdot y|),$$

and

$$d([x],[y]) = \min\{\cos^{-1}(x \cdot y), \pi - \cos^{-1}(x \cdot y)\}.$$

If the representatives $x, y \in \mathbb{R}^{n+1}$ of $p = [x]$ and $q = [q]$ are not unit vectors, then

$$d([x],[y]) = \cos^{-1}\left(\frac{|x \cdot y|}{\|x\| \, \|y\|}\right).$$

Note that $0 \leq d(p,q) \leq \pi/2$.

Now, the Euclidean distance between x and y on S^n is given by

$$\|x - y\|_2^2 = \|x\|_2^2 + \|y\|_2^2 - 2x \cdot y = 2 - 2\cos\theta = 4\sin^2(\theta/2).$$

Thus,

$$\|x - y\|_2 = 2\sin(\theta/2), \quad 0 \leq \theta \leq \pi.$$

It follows that for any $x \in S^n$, and for any subset $A \subseteq S^n$, a point $a \in A$ minimizes the distance $d_{S^n}(x,a) = \cos^{-1}(x \cdot a) = \theta$ on S^n iff it minimizes the Euclidean distance $\|x - a\|_2 = 2\sin(\theta/2)$ (since $0 \leq \theta \leq \pi$). Then, on $\mathbb{RP}^n$, for any point $p = [x] \in \mathbb{RP}^n$ and any $A \subseteq \mathbb{RP}^n$, a point $[a] \in A$ minimizes the distance $d([x],[a])$ on $\mathbb{RP}^n$ iff it minimizes $\min\{\|x - a\|_2, \|x + a\|_2\}$. So, we are looking for $[b] \in A$ such that

$$\begin{aligned} \min\{\|x - b\|_2, \|x + b\|_2\} &= \min_{[a] \in A} \min\{\|x - a\|_2, \|x + a\|_2\} \\ &= \min\{\min_{[a] \in A} \|x - a\|_2, \min_{[a] \in A} \|x + a\|_2\}. \end{aligned}$$

If the subset $A \subseteq S^n$ is closed under the antipodal map (which means that if $x \in A$, then $-x \in A$), then finding $\min_{a \in A} d([x],[a])$ on $\mathbb{RP}^n$ is equivalent to finding $\min_{a \in A} \|x - a\|_2$, the minimum of the Euclidean distance. This is the case for the set $\mathcal{X}$ in Section 4.2 and the set $\mathcal{K}$ in Section 4.3.

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