Chapter 18

Graphs and Graph Laplacians; Basic Facts

In this chapter and the next we present some applications of linear algebra to graph theory. Graphs (undirected and directed) can be defined in terms of various matrices (incidence and adjacency matrices), and various connectivity properties of graphs are captured by properties of these matrices. Another very important matrix is associated with a (undirected) graph: the *graph Laplacian*. The graph Laplacian is symmetric positive definite, and its eigenvalues capture some of the properties of the underlying graph. This is a key fact that is exploited in graph clustering methods, the most powerful being the method of normalized cuts due to Shi and Malik [58]. This chapter and the next constitute an introduction to algebraic and spectral graph theory. We do not discuss normalized cuts, but we discuss graph drawings. Thorough presentations of algebraic graph theory can be found in Godsil and Royle [28] and Chung [13].

We begin with a review of basic notions of graph theory. Even though the graph Laplacian is fundamentally associated with an undirected graph, we review the definition of both directed and undirected graphs. For both directed and undirected graphs, we define the degree matrix D, the incidence matrix B, and the adjacency matrix A. Then we 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:

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

The *degree matrix* is the diagonal matrix

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

The notion of degree is illustrated in Figure 18.1. Then we introduce the (unnormalized) *graph Laplacian* L of a directed graph G in an "old-fashion" way, by showing that for any

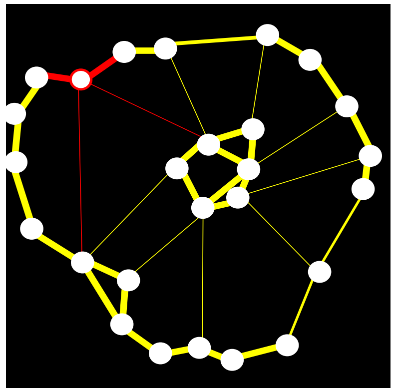

Figure 18.1: Degree of a node.

orientation of a graph G,

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

is an invariant. We also define the (unnormalized) *graph Laplacian* L of a weighted graph $G = (V, W)$ as $L = D - W$. We 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

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

We 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. We 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.

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

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

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, we turn to *graph drawings* (Chapter 19). 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

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

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 $w_{ij} \geq 0$. 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 [28], 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 we prove the main theorem about graph drawings (Theorem 19.2), 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 [60].

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

Definition 18.1. 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 18.2.

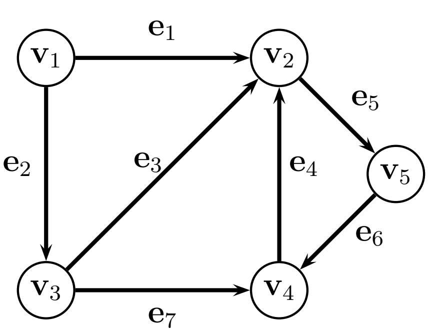

Figure 18.2: Graph G_1.

Definition 18.2. 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 18.3. 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 18.4. 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:

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

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

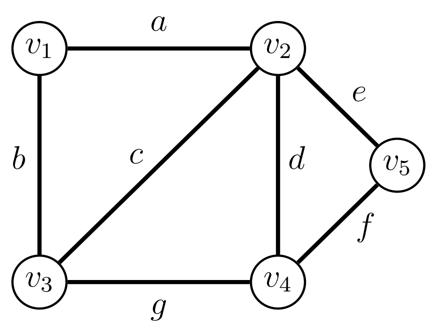

Figure 18.3: The undirected graph G_2.

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 18.5. 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 18.3.

Definition 18.6. 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 $D(G)$ (or simply, D) is defined as in Definition 18.2.

Definition 18.7. 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 18.8. 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 $B(G)$.

Definition 18.9. 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.

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

Definition 18.10. 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 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 18.11. 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 18.1. *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 [28], Section 8.3). The fact that $\mathrm{rank}(B) = m - c$ 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 $z \in \mathrm{Ker}\,(B^\top)$ 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 $\dim(\mathrm{Ker}\,(B^\top)) = c$, and that $\mathrm{Ker}\,(B^\top)$ has a basis consisting of indicator vectors.

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

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

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

Definition 18.12. Following common practice, we denote by $\mathbf{1}$ the (column) vector (of dimension m) 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 18.1, 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 $w_{i\,j}$ to an edge $\{v_i, v_j\}$; the smaller $w_{i\,j}$ is, the weaker is the link (or similarity) between v_i and v_j, and the greater $w_{i\,j}$ is, the stronger is the link (or similarity) between v_i and v_j.

Definition 18.13. 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 $w_{i\,j} \geq 0$ for all $i, j \in \{1, \ldots, m\}$, and $w_{i\,i} = 0$ for $i = 1, \ldots, m$. We say that a set $\{v_i, v_j\}$ is an edge iff $w_{i\,j} > 0$. The corresponding (undirected) graph (V, E) with $E = \{\{v_i, v_j\} \mid w_{i\,j} > 0\}$, is called the *underlying graph* of G.

Remark: Since $w_{i\,i} = 0$, these graphs have no self-loops. We can think of the matrix W as a generalized adjacency matrix. The case where $w_{i\,j} \in \{0, 1\}$ is equivalent to the notion of a graph as in Definition 18.5.

We can think of the weight $w_{i\,j}$ 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 18.4. The thickness of an edge corresponds to the magnitude of its weight.

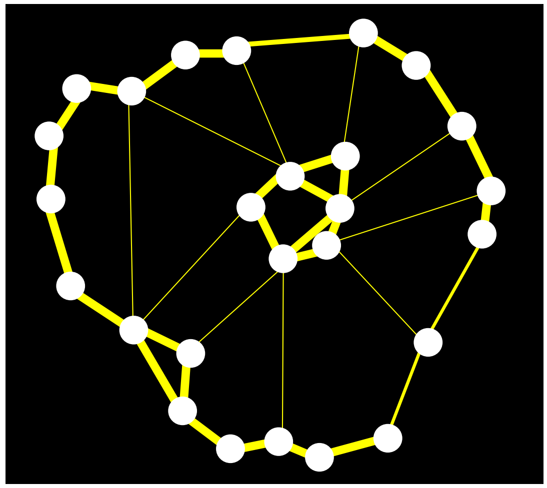

Figure 18.4: A weighted graph.

Definition 18.14. Given a weighted graph $G = (V, W)$, 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:

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

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 $D(G)$ (or simply, D) is defined as before, namely by $D(G) = \mathrm{diag}(d(v_1), \ldots, d(v_m))$.

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.

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

18.2 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 [24] (see also Godsil and Royle [28]).

Proposition 18.2. *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 $D_{i\,i} = d(v_i)$, 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 $B^\sigma (B^\sigma)^\top_{i\,j}$ is the inner product of the ith row b^σ_i, and the jth row b^σ_j 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 $b^\sigma_i \cdot b^\sigma_i = d(v_i)$. If $i \neq j$, then $b^\sigma_i \cdot b^\sigma_j \neq 0$ 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, $b^\sigma_i \cdot b^\sigma_j = -1$. 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 nonnegative. ∎

Definition 18.15. The matrix $L = B^\sigma (B^\sigma)^\top = D - A$ is called the *(unnormalized) graph Laplacian* of the graph G^σ. The *(unnormalized) graph Laplacian* of an undirected graph $G = (V, E)$ is defined by

$$L = D - A.$$

For example, the graph Laplacian of graph G_1 is

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

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 18.8), it can be shown that
$$BB^{\top} = D + A.$$

2. As pointed out by Evangelos Chatzipantazis, Proposition 18.2 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 18.16. 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 D instead of $D(G)$ and 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 from the equation $L = D - W$ 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 18.17. 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 18.3.

It is easy to see that Proposition 18.1 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 18.2 whose proof is immediately adapted.

Proposition 18.3. *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 G, 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.

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

Proposition 18.4. *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 (that is, $d_i = \sum_{j=1}^m w_{ij}$), then we have*

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

Consequently, $x^\top Lx$ 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.

Proof. We have

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

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

Proposition 18.4 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 18.5. *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 18.1, 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 $\mathrm{Ker}\,(L)$. $\square$

Proposition 18.5 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 [28] (Chapter 13) and Chung [13]. 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*.

18.3 Normalized Laplacian Matrices of Graphs

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.

Definition 18.18. Given a weighted graph $G = (V, W)$, a vertex $u \in V$ is *isolated* if it is not incident to any other vertex. This means that every row of W contains some strictly positive entry.

If G has no isolated vertices, then 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 18.19. 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.

Example 18.1. As an example, the matrices L_{sym} and L_{rw} associated with the graph G_1 are

$$L_{\mathrm{sym}} = \begin{pmatrix} 1.0000 & -0.3536 & -0.4082 & 0 & 0 \\ -0.3536 & 1.0000 & -0.2887 & -0.2887 & -0.3536 \\ -0.4082 & -0.2887 & 1.0000 & -0.3333 & 0 \\ 0 & -0.2887 & -0.3333 & 1.0000 & -0.4082 \\ 0 & -0.3536 & 0 & -0.4082 & 1.0000 \end{pmatrix}$$

and

$$L_{\text{rw}} = \begin{pmatrix} 1.0000 & -0.5000 & -0.5000 & 0 & 0 \\ -0.2500 & 1.0000 & -0.2500 & -0.2500 & -0.2500 \\ -0.3333 & -0.3333 & 1.0000 & -0.3333 & 0 \\ 0 & -0.3333 & -0.3333 & 1.0000 & -0.3333 \\ 0 & -0.5000 & 0 & -0.5000 & 1.0000 \end{pmatrix}.$$

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

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

we get

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

In particular, for any singular decomposition $B_{\text{sym}} = U\Sigma V^\top$ 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 $Lx = \lambda Dx$.

Proposition 18.6. *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,

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

(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 $u \in \text{Ker}\,(L)$ iff $D^{1/2}u \in \text{Ker}\,(L_{\text{sym}})$.

(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,*[1] *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

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

follows immediately from Proposition 18.4 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,

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

iff

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

iff

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

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

$$Lu = \lambda Du$$

iff

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

[1] Recall that an undirected graph is complete if for any two distinct nodes u, v, there is an edge $\{u, v\}$.

iff

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

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 $L_{\rm sym}$ for the eigenvalue λ. The second part of the statement follows from (2).

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

(6) Since $L\mathbf{1} = 0$, we get $L_{\rm rw}\mathbf{1} = D^{-1}L\mathbf{1} = 0$. That $D^{1/2}\mathbf{1}$ is in the nullspace of $L_{\rm sym}$ follows from (2). Properties (7)–(10) are proven in Chung [13] (Chapter 1). $\square$

The eigenvalues the matrices $L_{\rm sym}$ and $L_{\rm rw}$ from Example 18.1 are

$$0,\ 7257,\ 1.1667,\ 1.5,\ 1.6076.$$

On the other hand, the eigenvalues of the unormalized Laplacian for G_1 are

$$0,\ 1.5858,\ 3,\ 4.4142,\ 5.$$

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

A version of Proposition 18.5 also holds for the graph Laplacians $L_{\rm sym}$ and $L_{\rm rw}$. This follows easily from the fact that Proposition 18.1 applies to the underlying graph of a weighted graph. The proof is left as an exercise.

Proposition 18.7. *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 $L_{\rm sym}$ and $L_{\rm rw}$, which is equal to the multiplicity of the eigenvalue 0. Furthermore, the nullspace of $L_{\rm rw}$ 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 $L_{\rm sym}$, a basis of the nullpace is obtained by multiplying the above basis of the nullspace of $L_{\rm rw}$ by $D^{1/2}$.*

A particularly interesting application of graph Laplacians is graph clustering.

18.4 Graph Clustering Using Normalized Cuts

In order to explain this problem we need some definitions.

Definition 18.20. 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:

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

Given any two subsets $A, B \subseteq V$ (not necessarily distinct), we define links(A, B) by

$$\text{links}(A, B) = \sum_{v_i \in A, v_j \in B} w_{i\,j}.$$

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

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

The notion of volume is illustrated in Figure 18.5 and the notions of cut is illustrated in Figure 18.6.

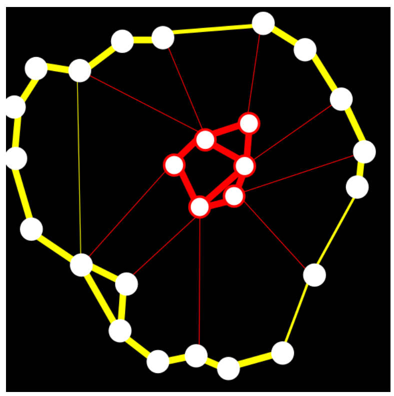

Figure 18.5: Volume of a set of nodes.

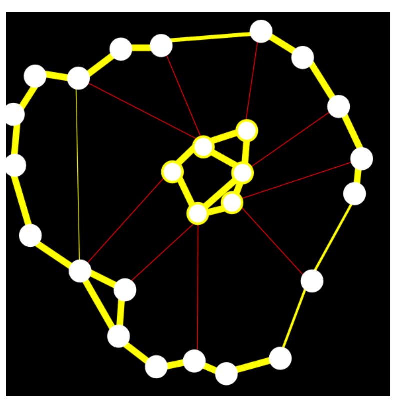

Figure 18.6: A cut involving the set of nodes in the center and the nodes on the perimeter.

The above concepts play a crucial role in the theory of normalized cuts. This beautiful and deeply original method first published in Shi and Malik [58], 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 [75] and is also the subject of Yu and Shi [76].

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 18.7.

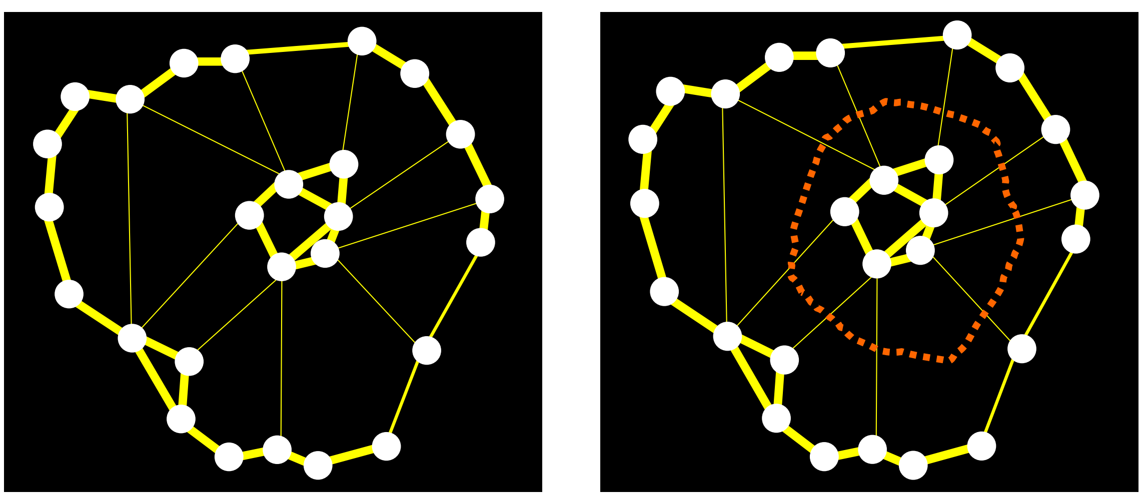

Figure 18.7: A weighted graph and its partition into two clusters.

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 [58]. Subsequently, Yu (in her dissertation [75]) and Yu and Shi [76] 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 next step is to express our optimization problem in matrix form, and this can be done in terms of Rayleigh ratios involving the graph Laplacian in the numerators. This theory is very beautiful, but we do not have the space to present it here. The interested reader is referred to Gallier [23].

18.5 Summary

The main concepts and results of this chapter are listed below:

- Directed graphs, undirected graphs.
- Incidence matrices, adjacency matrices.
- Weighted graphs.
- Degree matrix.
- Graph Laplacian (unnormalized).
- Normalized graph Laplacian.
- Spectral graph theory.
- Graph clustering using normalized cuts.

18.6 Problems

Problem 18.1. Find the unnormalized Laplacian of the graph representing a triangle and of the graph representing a square.

Problem 18.2. Consider the complete graph K_m on $m \geq 2$ nodes.

(1) Prove that the normalized Laplacian L_{sym} of K is

$$L_{\mathrm{sym}} = \begin{pmatrix} 1 & -1/(m-1) & \ldots & -1/(m-1) & -1/(m-1) \\ -1/(m-1) & 1 & \ldots & -1/(m-1) & -1/(m-1) \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ -1/(m-1) & -1/(m-1) & \ldots & 1 & -1/(m-1) \\ -1/(m-1) & -1/(m-1) & \ldots & -1/(m-1) & 1 \end{pmatrix}.$$

(2) Prove that the characteristic polynomial of L_{sym} is

$$\begin{vmatrix} \lambda-1 & 1/(m-1) & \dots & 1/(m-1) & 1/(m-1) \\ 1/(m-1) & \lambda-1 & \dots & 1/(m-1) & 1/(m-1) \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 1/(m-1) & 1/(m-1) & \dots & \lambda-1 & 1/(m-1) \\ 1/(m-1) & 1/(m-1) & \dots & 1/(m-1) & \lambda-1 \end{vmatrix} = \lambda\left(\lambda - \frac{m}{m-1}\right)^{m-1}.$$

Hint. First subtract the second column from the first, factor $\lambda - m/(m-1)$, and then add the first row to the second. Repeat this process. You will end up with the determinant

$$\begin{vmatrix} \lambda - 1/(m-1) & 1 \\ 1/(m-1) & \lambda - 1 \end{vmatrix}.$$

Problem 18.3. Consider the complete bipartite graph $K_{m,n}$ on $m+n \geq 3$ nodes, with edges between each of the first $m \geq 1$ nodes to each of the last $n \geq 1$ nodes. Prove that the eigenvalues of the normalized Laplacian L_{sym} of $K_{m,n}$ are 0 with multiplicity $m+n-2$ and 1 with multiplicity 2.

Problem 18.4. Let G be a graph with a set of nodes V with $m \geq 2$ elements, without isolated nodes, and let $L_{\mathrm{sym}} = D^{-1/2}LD^{-1/2}$ be its normalized Laplacian (with L its unnormalized Laplacian).

(1) For any $y \in \mathbb{R}^V$, consider the Rayleigh ratio

$$R = \frac{y^\top L_{\mathrm{sym}}\, y}{y^\top y}.$$

Prove that if $x = D^{-1/2}y$, then

$$R = \frac{x^\top L x}{(D^{1/2}x)^\top D^{1/2}x} = \frac{\displaystyle\sum_{u\sim v}(x(u)-x(v))^2}{\displaystyle\sum_v d_v x(v)^2}.$$

(2) Prove that the second eigenvalue ν_2 of L_{sym} is given by

$$\nu_2 = \min_{\mathbf{1}^\top Dx=0, x\neq 0} \frac{\displaystyle\sum_{u\sim v}(x(u)-x(v))^2}{\displaystyle\sum_v d_v x(v)^2}.$$

(3) Prove that the largest eigenvalue ν_m of L_{sym} is given by

$$\nu_m = \max_{x\neq 0} \frac{\displaystyle\sum_{u\sim v}(x(u)-x(v))^2}{\displaystyle\sum_v d_v x(v)^2}.$$

Problem 18.5. Let G be a graph with a set of nodes V with $m \geq 2$ elements, without isolated nodes. If $0 = \nu_1 \leq \nu_1 \leq \ldots \leq \nu_m$ are the eigenvalues of L_{sym}, prove the following properties:

(1) We have $\nu_1 + \nu_2 + \cdots + \nu_m = m$.

(2) We have $\nu_2 \leq m/(m-1)$, with equality holding iff $G = K_m$, the complete graph on m nodes.

(3) We have $\nu_m \geq m/(m-1)$.

(4) If G is not a complete graph, then $\nu_2 \leq 1$

Hint. If a and b are nonadjacent nodes, consider the function x given by

$$x(v) = \begin{cases} d_b & \text{if } v = a \\ -d_a & \text{if } v = b \\ 0 & \text{if } v \neq a, b, \end{cases}$$

and use Problem 18.4(2).

(5) Prove that $\nu_m \leq 2$. Prove that $\nu_m = 2$ iff the underlying graph of G contains a nontrivial connected bipartite component.

Hint. Use Problem 18.4(3).

(6) Prove that if G is connected, then $\nu_2 > 0$.

Problem 18.6. Let G be a graph with a set of nodes V with $m \geq 2$ elements, without isolated nodes. Let $\mathrm{vol}(G) = \sum_{v \in V} d_v$ and let

$$\overline{x} = \frac{\sum_v d_v x(v)}{\mathrm{vol}(G)}.$$

Prove that

$$\nu_2 = \min_{x \neq 0} \frac{\displaystyle\sum_{u \sim v} (x(u) - x(v))^2}{\displaystyle\sum_v d_v (x(v) - \overline{x})^2}.$$

Problem 18.7. Let G be a connected bipartite graph. Prove that if ν is an eigenvalue of L_{sym}, then $2 - \nu$ is also an eigenvalue of L_{sym}.

Problem 18.8. Prove Proposition 18.7.