CISC 271 Class 3

Graphs: The Laplacian Matrix

Text Correspondence: $\sim$

Main Concepts:

- *Degree matrix D of graph $\mathcal{G}$: diagonal matrix*
- *Laplacian matrix of graph $\mathcal{G}$: $L = D - A$*
- *Laplacian matrix is symmetric positive semidefinite*
- *Fiedler vector: eigenvector of second-smallest eigenvalue*
- *Binary cluster: vertices classified by sign of Fiedler vector*

In graph theory, a commonly used matrix is derived from the adjacency matrix. The *Laplacian matrix* is usually written as L, despite the fact that it is a symmetric matrix and is not a lower-triangular matrix. We can define the Laplacian matrix of a graph by using some of the extensions that are defined in the extra notes for Class 1. First, we will define the commonly used *degree matrix* by using the $\mathrm{diag}(\cdot)$ operator of Definition 1.13.

Definition: degree matrix of a graph

For any graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$ that has an adjacency matrix $A_{n\times n}(\mathcal{G})$, the *degree matrix* $D(\mathcal{G})$ is the $n \times n$ diagonal matrix that is defined as

$$D(\mathcal{G}) \stackrel{\text{def}}{=} \mathrm{diag}([A]\vec{1}) \tag{3.1}$$

The Laplacian matrix is most often defined as the difference between the degree matrix of Equation 3.1 and the adjacency matrix of Equation 2.3.

Definition: Laplacian matrix of a graph

For any graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$ that has an adjacency matrix $A_{n\times n}(\mathcal{G})$ and a degree matrix $D_{n\times n}(\mathcal{G})$, the *Laplacian matrix* $L(\mathcal{G})$ is the $n \times n$ matrix that is defined as

$$L(\mathcal{G}) \stackrel{\text{def}}{=} D(\mathcal{G}) - A(\mathcal{G}) \tag{3.2}$$

Observation: The graph that is used to define the Laplacian matrix is usually understood by context, so it is common to abbreviate Equation 3.2 as

$$L = D - A$$

Let us re-visit the graph $\mathcal{G}_1$ that is specified in Equation 2.1 and that has the adjacency matrix A_1 that is specified in Equation 2.4. The degree matrix D_1 for the graph $\mathcal{G}_1$ is

$$D_1 \stackrel{\text{def}}{=} \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{3.3}$$

The Laplacian matrix of the graph $\mathcal{G}_1$ is the difference between the degree matrix and the adjacency matrix, so

$$L_1 \stackrel{\text{def}}{=} D_1 - A_1 = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{3.4}$$

We previously observed that the graph $\mathcal{G}_1$ has two components, which are distinct subgraphs. We can easily verify that the Laplacian matrix for the graph $\mathcal{G}_1$ can be partitioned as diagonal blocks that are non-zero matrices and off-diagonal blocks that are zero matrices, so

$$L_1 = \begin{bmatrix} L_{1S1} & \mathbf{0} \\ \mathbf{0} & L_{1S2} \end{bmatrix} \tag{3.5}$$

Each diagonal block of the Laplacian matrix L_1, described in Equation 3.5, is a Laplacian matrix of a subgraph of $\mathcal{G}_1$.

We can also compute the Laplacian matrix for the graph $\mathcal{G}_2$ that is specified in Equation 2.2 and that has the adjacency matrix A_2 that is specified in Equation 2.5. Omitting the presentation of the degree matrix, the Laplacian matrix of the graph $\mathcal{G}_2$ is

$$L_2 \stackrel{\text{def}}{=} D_2 - A_2 = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 3 & -1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix} \tag{3.6}$$

Consider: re-ordering the vertices of the graph $\mathcal{G}_2$. From the diagram in Figure 2.3, we can see that the integer that is assigned to each vertex must be distinct but that there is no required order. An alternative graph $\mathcal{G}_5$ can be defined as

$$\mathcal{G}_5 \stackrel{\text{def}}{=} \begin{cases} \mathcal{V}_5 &= \{1\ 2\ 3\ 4\ 5\ 6\} \\ \mathcal{E}_5 &= \{(1\ 4)\ \ (1\ 5)\ \ (1\ 6)\ \ (6\ 2)\ \ (6\ 3)\} \end{cases} \tag{3.7}$$

The graph defined in Equation 3.7 can be drawn as shown in Figure 3.1. One way to partition the vertices of graph $\mathcal{G}_5$ is as $\mathcal{V}_L = \{1\ 2\ 3\}$ and $\mathcal{V}_R = \{4\ 5\ 6\}$.

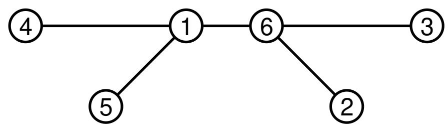

Figure 3.1: An illustration of the bipartite graph $\mathcal{G}_5$, having six vertices and five edges.

The adjacency matrix for graph $\mathcal{G}_5(\mathcal{V}_5, \mathcal{E}_5)$ is

$$A_5 = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix} \tag{3.8}$$

It is easy to see that the adjacency matrix A_5 of graph $\mathcal{G}_5$ can be partitioned into diagonal blocks that are zero matrices and off-diagonal blocks that are non-zero matrices, so that

$$A_5 = \begin{bmatrix} \mathbf{0} & A_{5S} \\ A_{5S}^T & \mathbf{0} \end{bmatrix} \tag{3.9}$$

3.1 Eigenvalues of a Laplacian Matrix

By definition, a Laplacian matrix is symmetric, real, and diagonally dominant. Such a matrix is guaranteed to be positive semidefinite, so its eigenvalues are non-negative. Let us explore these properties with some computational experiments.

Consider: multiplying a Laplacian matrix and a "ones" vector $\vec{1}$. As we discovered in the previous class, the resulting vector is the sum of the rows of the matrix. By definition, each diagonal entry of a Laplacian matrix is the sum of the corresponding row of the adjacency matrix, which is the degree of the graph. The remaining entries of each row of the Laplacian matrix are the negation of the corresponding row of the adjacency matrix. Consequently, the product of each row of a Laplacian matrix and the "ones" vector must be zero!

This can be verified for the above Laplacian matrices, for which we can compute

$$\begin{aligned} [L_1]\vec{1} &= \vec{0} \\ [L_2]\vec{1} &= \vec{0} \end{aligned} \tag{3.10}$$

We can see, from Equation 3.10, that the "ones" vector $\vec{1}$ must be an eigenvector of the Laplacian matrix, with the corresponding eigenvalue being $\lambda_1 = 0$.

Let us try a numerical experiment on the graph $\mathcal{G}_1$. If we use `MATLAB` to find the eigenvalues of the Laplacian matrix L_1, we find that these are approximately

$$\begin{aligned} \lambda_1 &= 0 \\ \lambda_2 &= 0 \\ \lambda_3 &= 2 \\ \lambda_4 &= 3 \\ \lambda_5 &= 3 \end{aligned}$$

<u>Observation:</u> The graph $\mathcal{G}_1$ has two components and there are two zero eigenvalues of the Laplacian matrix. In this case, the dimension of the nullspace of the Laplacian matrix is equal to the number of components.

If we are curious, we might want to see whether this is also true of graph $\mathcal{G}_3$, because it also has two components. The Laplacian matrix for graph $\mathcal{G}_3$ is

$$L_2 \stackrel{\text{def}}{=} D_2 - A_2 = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix} \tag{3.11}$$

By now we are unsurprised by the block structure of the Laplacian matrix L_3 in Equation 3.11 and we are keen to find its eigenvalues. Again using `MATLAB`, we get

$$\begin{aligned} \lambda_1 &= 0 \\ \lambda_2 &= 0 \\ \lambda_3 &= 2 \\ \lambda_4 &= 3 \\ \lambda_5 &= 3 \\ \lambda_6 &= 3 \end{aligned}$$

The pattern persists and we can consult external reference material to determine that this is a fact about the Laplacian matrix of a graph:

> *The dimension of the nullspace of the Laplacian matrix is equal to the number of components of the graph*

What can we discover by numerical experiments on our other graphs? We can try graph $\mathcal{G}_2$, which has eigenvalues that can be numerically approximated as

$$\begin{array}{lcl} \lambda_1 & = & 0 \\ \lambda_2 & \approx & 0.4384 \\ \lambda_3 & = & 2 \\ \lambda_4 & = & 3 \\ \lambda_5 & = & 3 \\ \lambda_6 & \approx & 4.5616 \end{array}$$

This is not especially fruitful, so let us examine one of the eigenvectors. The eigenvector for the second-smallest eigenvalue, λ_2, is approximately

$$\vec{v}_2 \approx \begin{bmatrix} -0.4647 \\ -0.2610 \\ -0.4647 \\ 0.2610 \\ 0.4647 \\ 0.4647 \end{bmatrix} \tag{3.12}$$

For the eigenvector $\vec{v}_2$ of Equation 3.12, the absolute values of the entries do not seem to be informative. However, the sign $(\pm)$ of the entries correspond to the visual clusters that we previously observed, which were $\{1\ \ 2\ \ 3\}$ and $\{4\ \ 5\ \ 6\}$. Is this true for the other clustered graph, $\mathcal{G}_4$?

Another graph that we have written is $\mathcal{G}_5$, which is a re-ordering of the graph $\mathcal{G}_2$. Doing the same computations, we find that eigenvalues and the eigenvector $\vec{v}_2$ are

$$\begin{array}{lcl} \lambda_0 & & \\ \lambda_2 & \approx & 0.4384 \\ \lambda_3 & = & 1 \\ \lambda_4 & = & 1 \\ \lambda_5 & = & 3 \\ \lambda_6 & \approx & 4.5616 \end{array} \qquad \vec{v}_2 \approx \begin{bmatrix} 0.2610 \\ -0.4647 \\ -0.4647 \\ 0.4647 \\ 0.4647 \\ -0.2610 \end{bmatrix} \tag{3.13}$$

The sign $(\pm)$ of the entries of $\vec{v}_2$ for graph $\mathcal{G}_5$ correspond to the visual clusters, which were $\{1\ \ 4\ \ 5\}$ and $\{2\ \ 3\ \ 6\}$.

3.2 The Fiedler Vector of a Graph

The eigenvector of the second-smallest eigenvalue is called the Fielder vector, named after Miroslav Fiedler who presented its use in 1989. His term for the property was “algebraic connectivity”.

Currently, the signs of the entries of the Fiedler vector are used as a *binary clustering* of a graph $\mathcal{G}$. The process for graph clustering is the same as we used in our numerical experiments above:

1. Compute the Laplacian matrix $L(\mathcal{G})$ of the graph $\mathcal{G}$
2. Compute the Fiedler vector as the eigenvector of the second-smallest eigenvalue
3. Determine the positive-negative sign of each entry
4. Assign negative entries to Set -1 and non-negative entries to Set +1

Now that we have many examples of how eigenvectors of a matrix can help us to analyze data, we will find it useful to explore the kinds of matrices to which we can apply these methods.

3.3 Extra Notes: Properties of a Laplacian Matrix

A Laplacian matrix $L(\mathcal{G})$ of a graph $\mathcal{G}$ has, among others, these properties:

- L is real and symmetric
- L is diagonally dominant
- From the above, L is positive semidefinite; written as $L \succeq 0$
- Both the row sum $[L]\vec{1}$ and the column sum $\vec{1}^T[L]$ are zero
- From the above, $\vec{1}$ is an eigenvector of the eigenvalue $\lambda_1 = 0$
- The number of connected components in the graph $\mathcal{G}$ is: (a) the dimension of the nullspace of the Laplacian matrix, which is the geometric multiplicity of the zero eigenvalue, and (b) is the algebraic multiplicity of the zero eigenvalue
- The eigenvector of the second-smallest eigenvalue, called the Fiedler vector, is a binary clustering of the vertices of the graph $\mathcal{G}$
- If the graph $\mathcal{G}$ has k components, then the Laplacian matrix of $\mathcal{G}$ is similar to a Laplacian matrix that has k non-zero diagonal blocks and zero off-diagonal blocks
- If the graph $\mathcal{G}$ is bipartite, then then the Laplacian matrix of $\mathcal{G}$ is similar to a Laplacian matrix that has two zero diagonal blocks and two non-zero off-diagonal blocks; from the above, the off-diagonal blocks are transposes of each other
- The trace of the Laplacian matrix, $\mathrm{tr}(L)$, is two times the number of edges in the graph $\mathcal{G}$

The Laplacian matrix is also closely related to the incidence matrix of a graph $\mathcal{G}$. For a graph $\mathcal{G}$ that has an adjacency matrix $A(\mathcal{G})$ as specified in Definition 2.3, a degree matrix $D(\mathcal{G})$ as specified in Definition 3.1, and an incidence matrix $C(\mathcal{G})$ as specified in Definition 2.12, a matrix identity is

$$L = 2D - CC^T \tag{3.14}$$

From the definition of the Laplacian matrix as $L = D - A$, the degree matrix can be deduced from the incidence as

$$D = \mathrm{diag}(\mathrm{diag}(CC^T)) \tag{3.15}$$

Combining Equation 3.14 and Equation 3.15, we can compute the adjacency matrix from the incidence matrix as

$$A = CC^T - D \tag{3.16}$$

