

AYUSHMAN ANUPAM (MDS202411) BISWAJIT KALA (MDS202412)

Boda Sowmya (MDS202413)

Data Science Chennai Mathematical Institute

Problem Statement

Motivation: Large graphical data structures can be difficult to store and process.

In case of tabular data, we can easily split it into multiple smaller tables. But what if the data is graphical and interconnected?

Challenge:

► How do we efficiently store, manage, and analyze large graph data?



Large Graph

Solution Overview

Solution Idea:

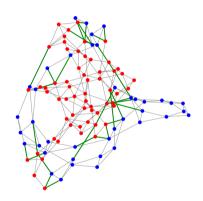
- Partition the large graph into smaller, manageable subgraphs.
- ► Store these subgraphs and record the relationships between them.

For this, we use a graph partitioning method called **Fiedler's Spectral Graph Partitioning**.

In this presentation, we will discuss:

- ► How it works
- Why it works (correctness)
- ► Implementation examples

Spectral Partitioning with Highlighted Cut Edges



Partitioned Graph Example

Abstract

- ▶ Solution focuses on dividing a connected graph *G* into two subgraphs to minimize the number of edges between them.
- ▶ It explores **spectral graph partitioning**, a method proposed by Fiedler using the Laplacian matrix and its eigenvectors. Vertices of *G* are split using one of the eigenvectors of the Laplacian matrix.
- ▶ Presentation conatins Fiedler's theorem claiming that subgraphs produced by this method are connected.
- ▶ Demonstrates the method on small example graphs to show how effectively it partitions them.

Introduction

Spectral graph partitioning partitions a graph into subgraphs satisfying the following properties:

- ▶ The partition divides the graph into two connected subgraphs.
- ▶ The number of vertices in each of the two subgraphs is nearly equal.
- ► The method minimizes the number of edges connecting the two subgraphs (i.e., the number of edges cut during partition).

Key points we are going to see:

- ► Partition is done using the **eigenvalues and eigenvectors** of the Laplacian matrix associated with the graph.
- ► The spectrum (eigenvalues) of a matrix determines the structure and properties of the partition.
- ▶ The paper presents Fiedler's technique to perform spectral graph partitioning.
- ▶ It restates the theorem that the subgraphs generated via spectral partitioning are connected.

Overview of Presentation

In this presentation, we aim to understand how spectral graph partitioning works by exploring the following key points:

- Graph Theory and Matrices associated to it.
- ▶ The **existence** of a suitable partition in any connected graph.
- A proof of how this method minimizes the loss of edges (information) between the subgraphs.
- ► The idea of a **partition line** (using eigenvectors) and why it effectively separates the graph.
- Demonstrating the connectedness of the resulting subgraphs after partitioning.
- Some Examples
- Application, limitations and future work

Introduction to Graph Theory

- ▶ A graph G = (V, E) is simple, undirected, and has Vertices V, Edges E connecting vertex pairs $(u, v) \in E$
- ▶ Vertices are labeled with unique integers 1, 2, ..., |V|.
- ▶ The **degree** of a vertex v, denoted d(v), is the number of edges incident on v.
- ▶ Adjacency Matrix $A(G) = (a_{i,j})$:

$$a_{i,j} = egin{cases} 1 & ext{if } (i,j) \in E \\ 0 & ext{otherwise} \end{cases}$$

▶ **Degree Matrix** $D(G) = (d_{i,j})$:

$$d_{i,j} = \begin{cases} d(i) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

▶ Laplacian Matrix: L(G) = D(G) - A(G)

Examples



Degree Matrix

D(G)

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Adjacency Matrix

A(G)

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

$$egin{bmatrix} 0 & 1 & 0 \ 1 & 0 & 1 \ 0 & 1 & 0 \ \end{bmatrix}$$

Laplacian Matrix

$$L(G) = D(G) - A(G)$$

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

$$\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

Eigenvalues and Eigenvectors of L(G)

- ▶ For $A \in \mathbb{R}^{n \times n}$ and a vector $\mathbf{x} \in \mathbb{R}^n$, if $A\mathbf{x} = \lambda \mathbf{x}$, then:
 - x is an eigenvector
 - \triangleright λ is the corresponding **eigenvalue**
- ightharpoonup An $n \times n$ matrix has at most n eigenvalue-eigenvector pairs.
- Repeated eigenvalues can occur, but with possibly different eigenvectors.
- Eigenvalues are solutions to:

$$\det(A - \lambda I_n) = 0$$

► Eigenvectors are found by solving:

$$(A - \lambda I_n)\mathbf{x} = \mathbf{0}$$

▶ **Note:** λ_1 (Smallest eigenvalue) of L(G) is always 0 and it is positive semi definite.

Method of Spectral Graph Partitioning

Fiedler's theory of spectral graph partitioning is based upon a very simple idea. For a graph G = (V, E) which is to be partitioned:

- ▶ The Laplacian matrix L(G) is formed.
- ▶ The eigenvalue-eigenvector pairs of L(G) are calculated.
- ▶ Label the eigenvalues so that $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.
- ▶ The eigenvector \mathbf{x}_2 , which corresponds to λ_2 (the second-smallest eigenvalue), is known as the *Fiedler vector*, and is used to partition the vertices.

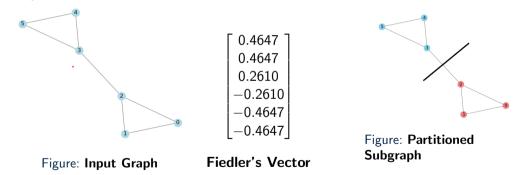
Let n = |V|. Recall:

- ▶ Each of the *n* vertices of *G* is assigned a unique label from the set $\{1, 2, ..., n\}$.
- ▶ $L(G) \in \mathbb{R}^{n \times n}$, and $\mathbf{x}_2 \in \mathbb{R}^n$.
- ► Therefore, each vertex corresponds to a single entry of \mathbf{x}_2 ; that is, vertex i corresponds to entry x_i in \mathbf{x}_2 .

To form the partition:

- ightharpoonup Create two graphs G_1 and G_2 .
- ▶ For each vertex $i \in G$, if $x_i < 0$, assign vertex i to G_1 ; otherwise, assign it to G_2 .

Examples 01



Examples 02

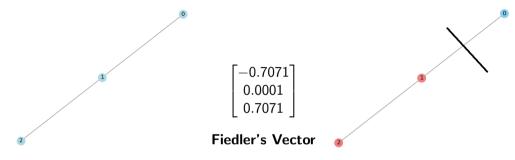


Figure: Input Graph

Figure: Partitioned Subgraph

This defines a partition of G into two sets. However, it is not evident that this partition minimizes the number of edges between G_1 and G_2 , or even that the two subgraphs are connected.

Why Second-Smallest Eigenvector — Standing Wave Analogy

To explain why Fiedler's partition works, we use the example of a vibrating string.

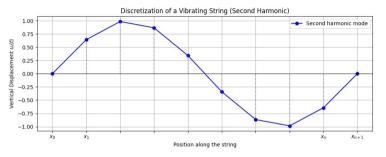


Figure: Illustration of a vibrating string

Consider a string of length L, discretized into n+1 equal segments, resulting in n interior points and two fixed boundary points at $x_0=0$ and $x_{n+1}=L$. Here, each x_i can be viewed as a vertex in a graph.

Note: The above is a *chain graph*, where each intermediate vertex has degree 2, and the two end vertices have degree 1. It represents a simple, linear sequence of connected vertices.

Segment length:

$$h = \frac{L}{n+1}, \quad x_i = i \cdot h, \quad i = 0, 1, \dots, n+1.$$

As $n \to \infty$, $h \to 0$ i.e, the discrete chain graph approaches a continuous string. This allows us to model the entire string as a chain graph. Relating this to the standing wave theory, we have:

- ▶ Vertical displacement at position x_i : $u_i(t)$.
- Fixed boundary conditions: $u_0(t) = 0$, $u_{n+1}(t) = 0$.
- ▶ Displacement vector for interior points:

$$\mathbf{u}(t) = \left[u_1(t), u_2(t), \vdots, u_n(t)\right]^t.$$

Note: Continuous wave equation $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$.

▶ In our case, Discrete second spatial derivative using central finite difference gives:

$$\frac{\partial^2 u_i}{\partial x^2} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}.$$

Writing it in matrix form foe all x_i gives matrix **D**:

$$\mathbf{D} = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 \end{bmatrix}.$$

which exactly looks like the Laplacian matrix of the chain graph.

► Substituting into the discrete wave equation:

$$\frac{d^2\mathbf{u}}{dx^2} \approx \frac{1}{h^2} \mathbf{D} \mathbf{u}$$

$$\implies \frac{d^2\mathbf{u}}{dt^2} = \frac{c^2}{h^2}\mathbf{D}\mathbf{u}$$

From the equation of a standing wave:

$$\frac{d^2\mathbf{u}}{dt^2} = -\omega^2\mathbf{u}$$

Comparing both, we arrive at the eigenvalue problem:

$$\mathbf{D}\mathbf{u} = -\frac{\omega^2 h^2}{c^2}\mathbf{u}$$

▶ **Note:** which is exactly the eigenvalue equation, with eigenvalue:

$$\lambda = \frac{-\omega^2 h^2}{c^2}$$

Note: The eigenvalues of **D** are given by:

$$\lambda_k = 2\left(1 - \cos\left(\frac{k\pi}{n+1}\right)\right), \quad k = 1, 2, \dots, n$$

where the eigenvalues are ordered as:

$$\lambda_1 < \lambda_2 < \cdots < \lambda_n$$

▶ The second smallest eigenvalue λ_2 is:

$$\lambda_2 = 2\left(1 - \cos\left(\frac{2\pi}{n+1}\right)\right)$$

▶ The corresponding natural frequency associated with λ_2 is:

$$\omega = 2\pi f = \sqrt{\frac{c^2 \lambda_2}{h^2}}$$

- The corresponding frequency f is equal to the second harmonic $\frac{c}{L}$ of the standing wave. This mode divides the particles of the string into two groups half with upward acceleration and half with downward acceleration. Similarly, the chain graph is partitioned into two parts with nearly equal numbers of vertices.
- From our earlier discussion, we observed that the second eigenvector of the Laplacian matrix L(G) partitions a chain graph into two nearly equal halves.
- ► For more complex graphs beyond simple chains, the same intuition holds. It is particularly intuitive in planar graphs, which can be visualized like a trampoline where the second mode of vibration similarly divides the graph (or trampoline) into two balanced regions.

Correctness of Partition - Mathematical View

Note:The smallest eigenvalue of L(G) is $\lambda_1 = 0$, and eigenvector associated with λ_1 is $\mathbf{v}_{\lambda_1} = [1, 1, \dots, 1]_{n \times 1}$.

Since smallest eigenvalue of L(G) is 0, we focus on the second smallest eigenvalue λ_2 .

$$\lambda_{2} = \min_{\mathbf{x} \perp \mathbf{1}} \frac{\mathbf{x}^{T} L \mathbf{x}}{\mathbf{x}^{T} \mathbf{x}}$$

$$= \min \sum_{i=1}^{n} \sum_{j=1}^{n} (D_{ij} - A_{ij}) x_{i} x_{j} = \sum_{i} D_{ii} x_{i}^{2} - 2 \sum_{(i,j) \in E} x_{i} x_{j}$$

$$= \min \sum_{(i,j) \in E} (x_{i}^{2} + x_{j}^{2} - 2x_{i} x_{j}) = \min \sum_{(i,j) \in E} (x_{i} - x_{j})^{2}$$

Note: Here, each x_i is associated with a node.

Since \mathbf{v}_{λ_1} and $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ are orthogonal eigenvectors:

$$\mathbf{v}_{\lambda_1}^T \mathbf{x} = \sum_{i=1}^n x_i = 0$$

Therefore:

- ightharpoonup Some labels x_i are negative, and some are positive.
- ► This naturally induces a partition of the graph into two sets:
 - ▶ Nodes with $x_i < 0$
 - ▶ Nodes with $x_i \ge 0$
- ▶ Hence, a **partition exists** based on the sign of the entries in the eigenvector corresponding to λ_2 .

So, the problem statement becomes:

$$\lambda_2 = \min_{ ext{all labelings of nodes s.t.}} \sum_{i} \sum_{x_i = 0} \sum_{(i,j) \in E} (x_i - x_j)^2$$

Note: The above summation is minimized when x_i and x_j have the same sign for each $(i,j) \in E$.

If they have different signs, the term $(x_i - x_j)^2$ increases, raising the overall summation.

This minimization ensures that the number of edges connecting nodes with different signs is as small as possible. In the context of graph partitioning:

- ▶ It minimizes the number of edges that are cut during the partition.
- Encourages connected nodes to remain within the same partition.

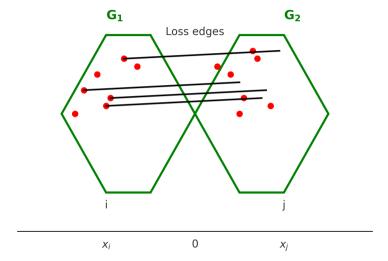
Balanced Partitioning Insight

Moreover: To minimize the above summation, we aim to reduce the total number of terms in the summation. Ideally, this is achieved when the number of vertices in both subgraphs is approximately equal.

Note: This condition does not always hold — it is a weak assumption. However, in most cases, balancing the number of vertices helps minimize the total number of possible (x_i, x_j) pairs across partitions, which effectively reduces the total cut value.

Hence, this method of partitioning ensures:

- ▶ The number of vertices in both partitions remains balanced.
- The number of edges cut between partitions is minimized.



Balance to minimize

what we did and Next Steps

So far, we have shown:

- ► A valid partition exists.
- ► The partition minimizes the number of lost (cut) edges.
- ▶ It ensures that the number of vertices in each subgraph is balanced.

What remains is to prove:

That the two subgraphs obtained from the partition are **connected**.

One of **Fiedler's key contributions** was proving that the two subgraphs formed through spectral partitioning are always connected.

Before presenting his proof, we will follow **Demmel's approach**, introducing some essential definitions and lemmas to build up the argument.

Some Linear Algebra Definition

Definition 1: Non-negative Matrix A matrix A is said to be *non-negative* if all of its elements are greater than or equal to zero, i.e.,

$$a_{ij} \geq 0$$
 for all i, j .

Definition 2: Spectral Radius The *spectral radius* of a square matrix A is the largest absolute value among its eigenvalues. It is denoted by:

$$\rho(A) = \max_{i} |\lambda_i|,$$

where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the matrix A.

Definition 3: Positive Definite Matrix A square matrix A is called *positive definite* if:

 $x^T A x > 0$ for all non-zero vectors x.

Remark 4: Symmetric and Positive-Definite Matrices The matrix *A* is symmetric and positive definite if and only if every eigenvalue of *A* is positive. In addition, *A* is symmetric and positive semi-definite if and only if every eigenvalue of *A* is nonnegative.

Lemmas and Theorem from Linear Algebra

Lemma 5. If A is an $n \times n$ symmetric matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$, then

$$\lambda_1 = \min_{v \neq 0} \frac{v^T A v}{v^T v}, \quad \lambda_n = \max_{v \neq 0} \frac{v^T A v}{v^T v}.$$

That is, λ_1 and λ_n are the minimum and maximum values of the expression $\frac{v^T A v}{v^T v}$ taken over all nonzero vectors $v \in \mathbb{R}^n$.

Proof. Let $v \in \mathbb{R}^n$ be any non-zero vector. Define the Rayleigh quotient:

$$R(v) = \frac{v^T A v}{v^T v}.$$

Let
$$y = \frac{v}{\|v\|}$$
, so $\|y\| = 1$, and thus $R(v) = y^T A y$.

Since A is symmetric, it is orthogonally diagonalizable. That is, $A = Q\Lambda Q^T$, where Q is an orthogonal matrix and $\Lambda = \text{diag}(\lambda_n \lambda_n \lambda_1)$. Then.

$$y^T A y = y^T Q \Lambda Q^T y = (Q^T y)^T \Lambda (Q^T y).$$

Let $z = Q^T y$, so ||z|| = ||y|| = 1. Then,

$$\frac{v^T A v}{v^T v} = z^T \Lambda z = \sum_{i=1}^n \lambda_{n-i+1} z_i^2 = z_1^2 \lambda_n + z_2^2 \lambda_{n-1} + \dots + z_n^2 \lambda_1,$$

Since $\sum_{i=1}^{n} z_i^2 = 1$, this is a convex combination of the eigenvalues λ_i . Therefore,

$$\lambda_1 \leq R(v) \leq \lambda_n$$
.

Hence,

$$\min_{v \neq 0} \frac{v^T A v}{v^T v} = \lambda_1, \quad \max_{v \neq 0} \frac{v^T A v}{v^T v} = \lambda_n.$$

Theorem 6 - Cauchy Interlacing Theorem

Cauchy Interlacing Theorem Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix with eigenvalues ordered as

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$$
.

Let A(i:i,i:i) denote the principal submatrix of A, formed by taking rows and columns *i* through *j*, so that $A(i:j,i:j) \in \mathbb{R}^{(j-i+1)\times(j-i+1)}$.

Let the eigenvalues of A(i:j, i:j) be

$$\chi_1 \leq \chi_2 \leq \cdots \leq \chi_{j-i+1}$$
.

Then for any k < j - i + 1, the matrix A has at least k eigenvalues that are less than or equal to χ_k ; that is,

$$|\{\lambda_{\ell} \mid \lambda_{\ell} \leq \chi_{k}\}| \geq k.$$

Cauchy Interlacing theorem simplified

▶ Consider any symmetric matrix A of size $n \times n$, with eigenvalues ordered as:

$$\lambda_n \geq \lambda_{n-1} \geq \cdots \geq \lambda_1$$

Let A_m be a submatrix of A of size $m \times m$ (with n > m) having eigenvalues:

$$\chi_m \geq \chi_{m-1} \geq \cdots \geq \chi_1$$

▶ Then for any $k \in \{1, 2, ..., m\}$, we must have at least k eigenvalues of A less than or equal to the k-th largest eigenvalue of A_m , that is:

$$|\{\lambda_{\ell} \mid \lambda_{\ell} \leq \chi_{k}\}| \geq k$$

Example: Cauchy Interlacing Theorem

Consider symmetric matrix A and its submatrix A_2 :

$$A = \begin{bmatrix} 4 & 1 & 0 & 0 \\ 1 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix}$$

Eigenvalues:

- ► For A: $\lambda = \{4.618, 3.382, 2, 1\}$
- ▶ For A_2 : $\chi = \{4.618, 2.382\}$

Check Interlacing:

- ▶ k = 2: $\chi_2 = 4.618 \ge \lambda_2 = 3.382 \ge \lambda_1 = 1$
- ▶ k = 1: $\chi_1 = 2.382 \ge \lambda_1 = 1$

Theorem 7

Let A be a $n \times n$ matrix and let X be any $n \times n$ non-singular matrix. Then X^TAX is symmetric positive-definite if and only if A is symmetric positive-definite.

Proof (\Leftarrow direction):

Assume *A* is symmetric positive definite. Then:

$$A = A^T$$
 and $\lambda_{\min}(A) > 0$

We analyze X^TAX :

1. Symmetry:

$$(X^T A X)^T = X^T A^T X = X^T A X$$
 (since $A = A^T$)

Therefore, X^TAX is symmetric.

2. Positive definiteness: Consider the Rayleigh quotient for X^TAX :

$$\lambda_{\min}(X^T A X) = \min_{v \neq 0} \frac{v^T X^T A X v}{v^T v}$$

Multiply and divide by $v^T X^T X v$ (valid for all $v \neq 0$):

$$= \min_{v \neq 0} \left(\frac{v^T X^T A X v}{v^T X^T X v} \cdot \frac{v^T X^T X v}{v^T v} \right)$$

Let y = Xv. Then:

$$\frac{v^T X^T A X v}{v^T X^T X v} = \frac{y^T A y}{y^T y} \ge \lambda_{\min}(A)$$

Also:

$$\frac{v^T X^T X v}{v^T v} \ge \lambda_{\min}(X^T X)$$

Hence:

$$\lambda_{\min}(X^T A X) \ge \lambda_{\min}(A) \cdot \lambda_{\min}(X^T X)$$

Since X is non-singular, X^TX is also non-singular, so $\lambda_{\min}(X^TX) > 0$. Therefore, $\lambda_{\min}(X^TAX) > 0$, and so X^TAX is positive definite. Thus, X^TAX is symmetric and positive definite.

$(\Longrightarrow direction)$

Assume X^TAX is symmetric positive definite. Then:

$$\lambda_{\min}(X^TAX) > 0$$

1. Symmetry: X^TAX is symmetric:

$$(X^T A X)^T = X^T A^T X$$

Since $X^TAX = X^TA^TX$, we conclude that $A = A^T$. Therefore, A is symmetric.

2. Positive definiteness: From earlier, we know:

$$\lambda_{\min}(X^T A X) = \lambda_{\min}(A) \cdot \lambda_{\min}(X^T X)$$

Since X is nonsingular, X^TX is also nonsingular, implying $\lambda_{\min}(X^TX) > 0$. For the product $\lambda_{\min}(X^TAX) = \lambda_{\min}(A) \cdot \lambda_{\min}(X^TX)$ to be positive, it follows that $\lambda_{\min}(A) > 0$. Therefore, A is positive definite.

Conclusion:

A is symmetric positive definite $\iff X^TAX$ is symmetric positive definite (when X is non singular).

Lemma 8

Let A be an $n \times n$ symmetric matrix. If $\rho(A) < 1$, meaning that all eigenvalues of A is on the interval (-1,1), then $I_n - A$ is nonsingular and:

$$(I_n - A)^{-1} = \sum_{i=0}^{\infty} A^i$$

Proof.

▶ Eigenvalues of $I_n - A$:

Since A is symmetric, its eigenvalues are real and lie in (-1,1). The identity matrix I_n has eigenvalues equal to 1. Hence, the eigenvalues of $I_n - A$ are:

$$\lambda_i(I_n-A)=1-\lambda_i(A)\in(0,2)$$

Therefore, all eigenvalues of $I_n - A$ are positive, which implies it is nonsingular.

► Convergence of the series:

Since A is symmetric, we can diagonalize it: $A = Q\Lambda Q^T$ where Q is orthogonal and Λ is diagonal.

Then: $A^i = Q\Lambda^iQ^T$ Since all $|\lambda_i| < 1$, $\Lambda^i \to 0$ as $i \to \infty$, and so: $A^i \to 0$ Thus, the series $\sum_{i=0}^{\infty} A^i$ converges.

► Telescoping sum argument:

Let $S_m = \sum_{i=0}^m A^i$. Then:

$$(I_n - A)S_m = (I_n - A)(I_n + A + \cdots + A^m) = I_n - A^{m+1}$$

As $m \to \infty$, $A^{m+1} \to 0$, so:

$$(I_n - A) \cdot \sum_{i=0}^{\infty} A^i = I_n$$

Therefore,
$$(I_n - A)^{-1} = \sum_{i=0}^{\infty} A^i$$

Fiedler's Theorem of Spectral Graph Partitioning

Let G be a connected graph and let L(G) be its Laplacian matrix. Create the subgraphs G_1 and G_2 using Fiedler's method. Then, both G_1 and G_2 are connected.

Proof (by contradiction):

- ightharpoonup Assume Without loss of generality G_1 is composed of two connected components.
- ▶ Let **x** be the eigenvector corresponding to λ_2 , the second-smallest eigenvalue of L(G).
- ▶ So both L(G) and **x** can be written in block form:

$$L(G) = \begin{bmatrix} L_{1,1} & O & L_{1,3} \\ O & L_{2,2} & L_{2,3} \\ L_{1,3}^T & L_{2,3}^T & L_{3,3} \end{bmatrix} \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix}$$

▶ Here, \mathbf{x} is the Fiedler vector (associated with λ_2) where \mathbf{x}_1 and \mathbf{x}_2 are positive and \mathbf{x}_3 is negative.

Proof of Fiedler's Theorem (continued)

- ▶ O denotes a matrix of appropriate size with all entries equal to zero.
- Note: L(G) is symmetric. Its Diagonal blocks of are symmetric and off-diagonal block in position (i, j) is the transpose of the block in position (j, i). Also, all off-diagonal blocks are non-positive.
- ▶ But, Each block $L_{i,j}$ has same properties, this implies, each Laplacian matrix, corresponds to subgraphs or components of the graph G.
- ▶ Since, graph is partitioned using the Fiedler vector \mathbf{x} . so, Vertices corresponding to \mathbf{x}_1 and \mathbf{x}_2 are grouped into the same subgraph G_1 .
- ▶ There are no edges between \mathbf{x}_1 and \mathbf{x}_2 , Since, the entries in L(1,2) and L(2,1) are 0. which implies: G_1 is disconnected and its components are represented by Laplacians like $L_{1,1}$ and others.

▶ Let **x** be an eigenvector of L(G) with eigenvalue λ_2 , so:

$$L(G)\mathbf{x}=\lambda_2\mathbf{x}.$$

 \triangleright Consider the first block \mathbf{x}_1 of \mathbf{x} . Multiplying out the corresponding block row:

$$L_{1,1}\mathbf{x}_1 + L_{1,3}\mathbf{x}_3 = \lambda_2\mathbf{x}_1.$$

- ▶ Since all eigenvalues of L(G) are nonnegative and by the **Cauchy Interlacing Theorem**, all eigenvalues of $L_{1,1}$ are also nonnegative.
- ▶ Let $\varepsilon > 0$. Add $\varepsilon \mathbf{x}_1$ to both sides of the equation:

$$\varepsilon \mathbf{x}_1 + L_{1,1}\mathbf{x}_1 + L_{1,3}\mathbf{x}_3 = \varepsilon \mathbf{x}_1 + \lambda_2 \mathbf{x}_1.$$

► This can be written more concisely as:

$$(\varepsilon I + L_{1,1})\mathbf{x}_1 + L_{1,3}\mathbf{x}_3 = (\varepsilon + \lambda_2)\mathbf{x}_1,$$

where I is the identity matrix of appropriate size.

▶ $L_{1,1}$ represents a subgraph of G, so its smallest eigenvalue is ≥ 0 . So, by the properties of I and symmetric matrices, and as discussed in the proof of Lemma 2.8, the eigenvalues of $\varepsilon I + L_{1,1}$ are all at least ε , hence:

$$\varepsilon I + L_{1,1}$$
 is positive-definite.

▶ Using Demmel's method, let:

$$\varepsilon I + L_{1,1} = D - N$$
,

where:

- ▶ D is diagonal, with each diagonal entry equal to the corresponding diagonal element of $\varepsilon I + L_{1,1}$,
- ▶ -L contains the off-diagonal entries of $\varepsilon I + L_{1,1}$,
- \blacktriangleright Every diagonal entry of -L is 0.

▶ This expression can be further decomposed as:

$$D^{\frac{1}{2}}\left(I-(D^{\frac{1}{2}})^{-1}N(D^{\frac{1}{2}})^{-1}\right)D^{\frac{1}{2}},$$

where $D^{\frac{1}{2}}$ is the matrix formed by taking the square root of each element of D.

► Since *D* is diagonal and nonnegative, we have:

$$D^{\frac{1}{2}}D^{\frac{1}{2}}=D.$$

► Multiply through the decomposition to verify:

$$\varepsilon I + L_{1,1} = D - N$$
.

Let:

$$M = (D^{\frac{1}{2}})^{-1}N(D^{\frac{1}{2}})^{-1},$$

which implies,

$$\varepsilon I + L_{1,1} = D - N = D^{\frac{1}{2}}(I - M)D^{\frac{1}{2}}.$$

► Since $D^{\frac{1}{2}}$ is diagonal, we have:

$$\left(D^{\frac{1}{2}}\right)^T = D^{\frac{1}{2}}.$$

► From Lemma 2.7 and earlier decomposition:

$$\varepsilon I + L_{1,1} = D^{\frac{1}{2}} (I - M) D^{\frac{1}{2}} \Rightarrow (D^{\frac{1}{2}})^T (I - M) D^{\frac{1}{2}}$$
 is positive-definite.

- ightharpoonup Thus, I-M is also positive-definite.
- Using symmetry arguments for eigenvalues:

If λ is an eigenvalue of M, then $1 - \lambda$ is an eigenvalue of I - M.

$$\implies 1 \geq \lambda_M$$

▶ From Lemma 2.5

$$egin{aligned} \lambda_1(M) &= \min_{\mathbf{v}
eq 0} rac{\mathbf{v}^T M \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \ &\Longrightarrow \ \lambda_1(M) \geq \min_{\mathbf{v}
eq 0} rac{-|\mathbf{v}|^T M |\mathbf{v}|}{\mathbf{v}^T \mathbf{v}} \geq \lambda_{n1}(M) = -\max_{\mathbf{v}
eq 0} rac{|\mathbf{v}|^T M |\mathbf{v}|}{\mathbf{v}^T \mathbf{v}} \ &\Longrightarrow \ \lambda_1(M) \geq -\lambda_{n_1}(M) > -1 \end{aligned}$$

where n_1 is the number of elements in x_1 .

▶ Hence, all eigenvalues of $M \in (1, -1)$

Now Assume for the sake of simplicity, $Y = (\varepsilon I + L_{1,1})^{-1}$

Recall that
$$\varepsilon \mathit{I} + \mathit{L}_{1,1} = \mathit{D}^{\frac{1}{2}}(\mathit{I} - \mathit{M})\mathit{D}^{\frac{1}{2}}.$$

$$\implies Y = (D^{\frac{1}{2}}(I - M)D^{\frac{1}{2}})^{-1} = (D^{\frac{1}{2}})^{-1}(I - M)^{-1}(D^{\frac{1}{2}})^{-1}.$$

So, by Lemma 2.8

$$(I-M)^{-1} = \sum_{i=0}^{\infty} M^i,$$

so

$$Y = (D^{\frac{1}{2}})^{-1} \left(\sum_{i=0}^{\infty} M^{i}\right) (D^{\frac{1}{2}})^{-1}.$$

▶ Since, M is nonnegative, $D^{\frac{1}{2}}$ is positive, M is symmetric and describes a graph,

 \implies M is positive and so is matrix Y is nonnegative

► Recall that:

$$(\varepsilon I + L_{1,1})\mathbf{x}_1 + L_{1,3}\mathbf{x}_3 = (\varepsilon + \lambda_2)\mathbf{x}_1.$$

► Multiplying both sides by *Y* gives:

$$\mathbf{x}_1 + YL_{1,3}\mathbf{x}_3 = (\varepsilon + \lambda_2)Y\mathbf{x}_1$$
, since $Y(\varepsilon I + L_{1,1}) = I$

► Multiplying by \mathbf{x}_1^T :

$$\mathbf{x}_1^T \mathbf{x}_1 + \mathbf{x}_1^T Y L_{1,3} \mathbf{x}_3 = (\varepsilon + \lambda_2) \mathbf{x}_1^T Y \mathbf{x}_1.$$

▶ Let n_1 be the number of elements in vector \mathbf{x}_1 . Then, using Lemma 2.5:

$$\begin{split} (\varepsilon + \lambda_2) \lambda_{n_1}(Y) &= \max_{\mathbf{v} \neq 0} \left((\varepsilon + \lambda_2) \cdot \frac{\mathbf{v}^T Y \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \right) \\ &\geq (\varepsilon + \lambda_2) \cdot \frac{\mathbf{x}_1^T Y \mathbf{x}_1}{\mathbf{x}_1^T \mathbf{x}_1} \\ &= \frac{\mathbf{x}_1^T \mathbf{x}_1 + \mathbf{x}_1^T Y L_{1,3} \mathbf{x}_3}{\mathbf{x}_1^T \mathbf{x}_1} \\ &= 1 + \frac{\mathbf{x}_1^T Y L_{1,3} \mathbf{x}_3}{\mathbf{x}_1^T \mathbf{x}_1} \end{split}$$

▶ The vector $L_{1,3}$ **x**₃ is positive, since $L_{1,3}$ is nonpositive, **x**₃ is negative, and if $L_{1,3}$ were zero, the graph G would not be connected.

 \implies Both the matrix Y and the vector \mathbf{x}_1 are positive.

$$\implies \mathbf{x}_1^T Y L_{1,3} \mathbf{x}_3$$
 is positive.

- ightharpoonup Also, $\mathbf{x}_1^T \mathbf{x}_1$ is positive.
- ► So from the previous inequality:

$$(\varepsilon + \lambda_2)\lambda_{n_1}(Y) > 1$$

 \implies All eigenvalues of Y are positive

- ▶ Since, all eigenvalues of Y are positive, and since $Y = (\varepsilon I + L_{1,1})^{-1}$, the eigenvalues of Y are the reciprocals of those of $\varepsilon I + L_{1,1}$.
- ▶ Hence, the largest eigenvalue of Y is the reciprocal of the smallest eigenvalue of $\varepsilon I + L_{1,1}$.

► Therefore:

$$\frac{\varepsilon + \lambda_2}{\lambda_1(\varepsilon I + L_{1,1})} > 1$$

Using the property:

$$\lambda_1(\varepsilon I + L_{1,1}) = \varepsilon + \lambda_1(L_{1,1}),$$

we get:

$$\frac{\varepsilon + \lambda_2}{\varepsilon + \lambda_1(L_{1,1})} > 1$$

► Rearranging the inequality:

$$\lambda_1(L_{1,1}) < \lambda_2$$

- ▶ Repeating similar steps for $L_{2,2}$, we get $\lambda_1(L_{2,2}) < \lambda_2$
- ► Currently, we have $\lambda_1(L_{1,1})$, $\lambda_1(L_{2,2}) < \lambda_2$

Finally, Consider the block matrix:

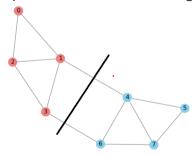
$$B = \begin{bmatrix} L_{1,1} & O \\ O & L_{2,2} \end{bmatrix}$$

Matrix B is a submatrix of L(G), so is Laplacian for some subgraph of G

- ▶ But by the Cauchy Interlacing Theorem $\lambda_2(L(G)) \leq \lambda_2(B)$.
- ▶ But from our calculation we found that $\lambda_1(L_{1,1})$, $\lambda_1(L_{2,2}) < \lambda_2$ i.e, $\lambda_2(L(G)) > \lambda_2(B)$ Which is a contradiction to **Cauchy Interlacing Theorem** \implies the original assumption must be false.
- ▶ Thus, G_1 is connected.
- ▶ Since, we proved for any general subgraph G_1 , our proof works of any subgraph of G.
- Theorem holds.

Implementation Spectral Partitioning Result

All implementation were done using Python, **Example 01**



Spectral Partitioned Graph

Laplacian Matrix:

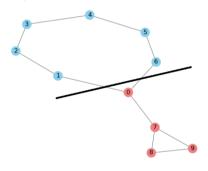
$$\begin{bmatrix} 2 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & 0 & -1 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 4 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & -1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

Fiedler Vector:

[0.4886, 0.2503, 0.1953, 0.4006, -0.2503, -0.4886, -0.4006, -0.1953]

Lost Edges between G_1 and G_2 : 2

Example 02



Spectral Partitioned Graph

Laplacian Matrix:

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

Fiedler Vector:

 $\left[0.0521, -0.1147, -0.2543, -0.3335, -0.3335, -0.2543, -0.1147, 0.3734, 0.4897, 0.4897\right]$

Lost Edges between G_1 and G_2 : 2

Industrial Applications

- Community Detection: Identify clusters in social or information networks.
- ▶ Image Segmentation: Partition images into regions based on similarity.
- Web Graph Analysis: Analyze internet topology or hyperlink networks.
- Biological Networks: Discover functional modules in gene or protein networks.
- ▶ **VLSI Design:** Efficiently partition circuits for chip design.
- ▶ Parallel Computing: Divide tasks while minimizing inter-process communication.

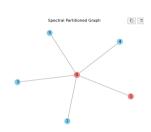
Limitations of Spectral Partitioning

Although Fiedler's Spectral Partitioning works well in many cases, it has limitations:

Examples of cases where it struggles:

- Star Graph: A graph with one central vertex connected to all others (as shown in figure).
 Since, removing central edge removes all edges and graph becomes disconnected
- Graphs with highly skewed degree distributions.
- Graphs where edge density is unevenly concentrated.

Why it fails: In these cases, the second smallest eigenvalue (Fiedler value) and the corresponding eigenvector may not produce a balanced or meaningful partition.



Star Graph Example

Further Work after Fiedler's Decomposition

- ► **Multiway Spectral Clustering:** Use multiple eigenvectors (beyond the second smallest) for *k*-way graph partitioning.
- ► **Graph Coarsening:** Combine with graph reduction techniques (like collapsing and merging) to simplify large graphs for efficient computations.
- ▶ **Dynamic Graphs:** Combine other methods like anomaly detection and then apply Fiedler decomposition.
- ► **Spectral Embedding:** Use multiple eigenvectors to embed graphs in 2D/3D for visualization and pattern discovery.
- ► **Graph Signal Processing:** Treat Fiedler vector as a low-frequency graph signal for tasks like denoising and filtering.

Conclusion

- ▶ We explored the theory and application of **Spectral Graph Partitioning** using the **Fiedler vector**.
- ▶ The graph Laplacian L(G) was constructed from the adjacency and degree matrices of each graph.
- ► The **second smallest eigenvector** of the Laplacian, known as the Fiedler vector, was used to divide the graph into two meaningful partitions.
- Example graphs demonstrated that this approach is both interpretable and effective in detecting natural partitions.
- Visualizations of graphs and their matrix forms validated the partitioning process.

References

- Spectral Graph Partitioning Finding a Partition (YouTube)
- ▶ James Demmel. Graph Partitioning, Part 1. Available at: http://www.cs.berkeley.edu/~demmel/cs267/lecture18/lecture18.html (1996)
- ▶ James Demmel. Graph Partitioning, Part 2. Available at: http://www.cs.berkeley.edu/~demmel/cs267/lecture20/lecture20.html (1999)
- ▶ Basic Graph Theory GeeksForGeeks: https://www.geeksforgeeks.org/fundamentals-of-graph-theory/
- ► All resources are available at: https://github.com/AyushmanGHub/ Fiedlers-Spectral-Graph-Partitioning-Paper/