Introduction to Spectral Graph Theory

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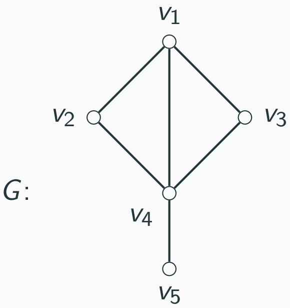
Outline

Spectral graph theory intertwines the field of graph theory with linear algebra by studying a graph's connectivity and structure.

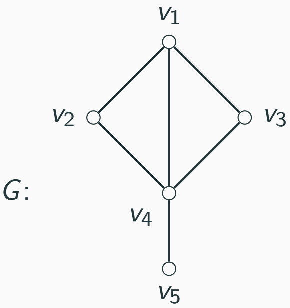
- **Introduction to Graphs**
- **The Adjacency Matrix**
- **The Incidence Matrix**
- **The Graph Laplacian**
- **Eigenvalues & Eigenvectors**
- **Graph Partitioning**

What is a Graph?



- $G = (V, E)$ where V is the vertex set, E is the edge set.
- Edge $e \in E$ is a pair uv of distinct vertices $u, v \in V$.

What is a Graph?



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- Edge $e \in E$ is a pair uv of distinct vertices $u, v \in V$.
    - $V = \{v_1, v_2, v_3, v_4, v_5\}$
    - $E = \{v_1v_2, v_1v_3, v_1v_4, v_2v_3, v_4v_3, v_3v_5\}$

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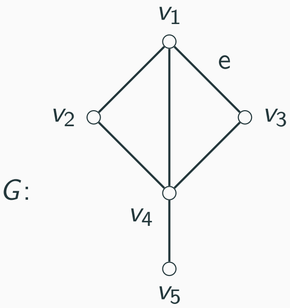

- Vertices u, v are **adjacent** if $uv \in E$.
- Vertex u and edge e are **incident** if $e = uv \in E$.
- **Degree** $\deg v$ is the $\#$ of edges incident to v.

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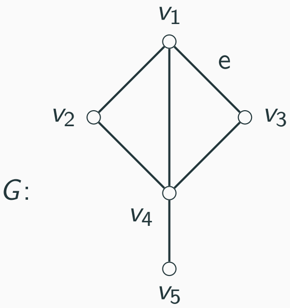

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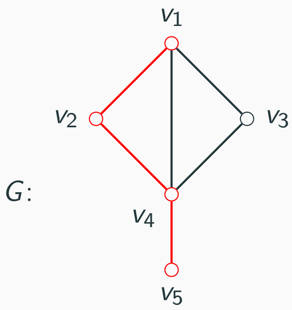
- **Degree** deg v is the # of edges incident to v.
- v_1 and v_2 are adjacent.
- v_1 and edge $e = v_1 v_3$ are incident.
- $\deg(v_4) = 4$.

Properties of Graphs



- $u - v$ walk: starts at u, goes to adjacent vertex, repeat until vertex v.
  - One possible $v_1 - v_5$ walk is $\{v_1, v_2, v_4, v_5\}$.
- A graph is **connected** if every pair of vertices is connected by a walk.

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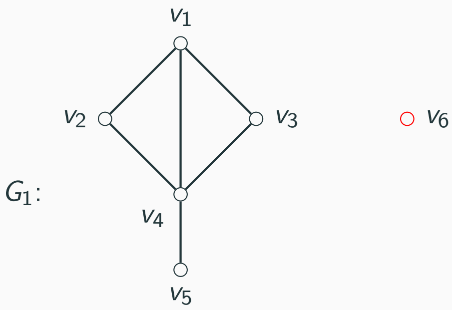

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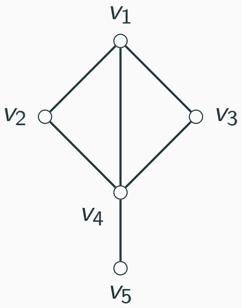
The Adjacency Matrix

Definition: For a graph G with n vertices, the adjacency matrix A is the $n \times n$ symmetric matrix with $A_{ij} = 1$ when $v_i v_j \in E$. Otherwise, $A_{ij} = 0$.

G:

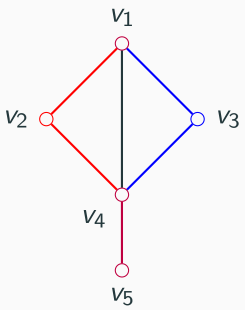


$$\mathrm{A} = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Powers of the Adjacency Matrix

Theorem: The element $(A^n)_{ij}$ is the number of unique $v_i - v_j$ walks of length n. Example: $A^3_{v_1 v_5} = 2$.

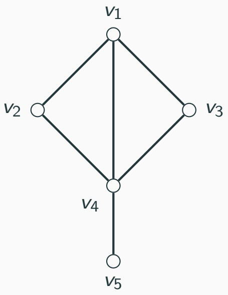
G:



$$A^3 = \begin{bmatrix} 4 & 5 & 5 & 6 & 2 \\ 5 & 2 & 2 & 6 & 1 \\ 5 & 2 & 2 & 6 & 1 \\ 6 & 6 & 6 & 4 & 4 \\ 2 & 1 & 1 & 4 & 0 \end{bmatrix}$$

Adjacency Matrix and Its Powers

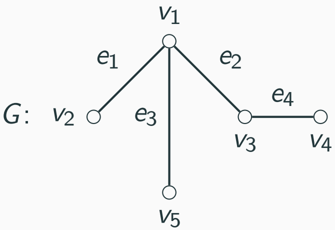
$$A = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad A^2 = \begin{bmatrix} 3 & 1 & 1 & 2 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 1 & 2 & 2 & 1 & 1 \\ 2 & 1 & 1 & 4 & 0 \\ 1 & 1 & 1 & 0 & 1 \end{bmatrix} \quad A^3 = \begin{bmatrix} 4 & 5 & 5 & 6 & 2 \\ 5 & 2 & 2 & 6 & 1 \\ 5 & 2 & 2 & 6 & 1 \\ 6 & 6 & 6 & 4 & 4 \\ 2 & 1 & 1 & 4 & 0 \end{bmatrix}$$



$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 1 \\ 1 \\ 2 \\ 1 \end{bmatrix} = 1 \cdot 1 + 1 \cdot 1 = 2$$

The Incidence Matrix

Definition: For a graph G with n vertices and m edges, the incidence matrix B is the $n \times m$ matrix with $B_{ij} = 1$ if v_i is incident with e_j. Otherwise, $B_{ij} = 0$.



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

The Graph Laplacian

The **graph Laplacian** (or Laplacian matrix) is a powerful way to observe **connectivity** and relationships between vertices and edges in graphs.

The graph Laplacian is a discrete **Laplace operator**. So what does the Laplace operator do?

The Laplace operator of a point on a function takes the **difference** between the value of that point and the average of the points that surround it.

The graph Laplacian is an application of the Laplace operator; it compares a vertex to those adjacent to it.

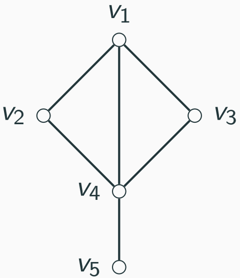
Definition of the Graph Laplacian

Definiton: $L = D - A$.

- D is the **degree** matrix.

- A is the **adjacency** matrix.

Alternate definition: $L = BB^T$.

G: 

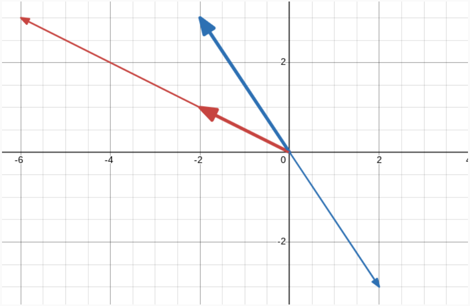
$$L = \begin{bmatrix} 3 & -1 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 & 0 \\ -1 & 0 & 2 & -1 & 0 \\ -1 & -1 & -1 & 4 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

Eigenvalues and Eigenvectors

Eigenvectors are special vectors such that when a transformation matrix is applied, the resulting vector is simply a scaled version of the original vector. The factor by which it is scaled is the *eigenvalue*.

Definition: The vector $\vec{v}$ is an eigenvector of a matrix A with eigenvalue λ if $A\vec{v} = \lambda\vec{v}$.

Eigenvalues and Eigenvectors - Example



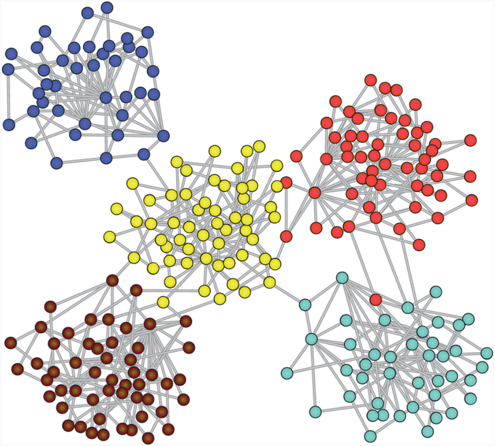
$$A = \begin{bmatrix} 5 & 4 \\ -3 & -3 \end{bmatrix}$$

$\lambda_1 = 3$ and $\lambda_2 = -1$

$\vec{v}_1 = [-2, 1]^T$ and $\vec{v}_2 = [-2, 3]^T$

What Am I Looking At?

Pretend we had a whole community of users on a social media platform. How would we arrange them by their friend groups?



Graph Partitioning Using the Graph Laplacian

The **Fiedler eigenvalue** is the second smallest eigenvalue of the Laplacian matrix of a graph. It determines the overall connectivity of the graph. The Fiedler Eigenvalue is greater than 0 iff G is connected.

Fiedler's method of **spectral partitioning** splits a graph: keeps the # of vertices the same while minimizing connections between the two partitions.

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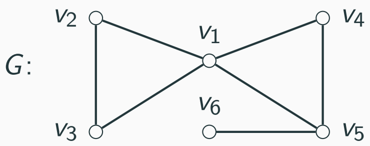
1. Find the Laplacian matrix of the graph.

2. Find the Fiedler eigenvalue λ and the Fiedler eigenvector μ of the graph.

3. For every $v_i \in G$: if $\mu_i < 0$, then v_i is partitioned into G_1. Otherwise, partitioned into G_2.

Example with Graph Partitioning



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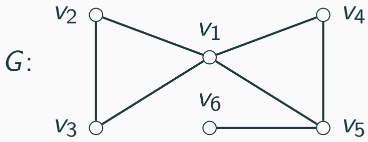

First Step: Calculating the Laplacian Matrix of the Graph.

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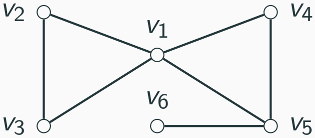

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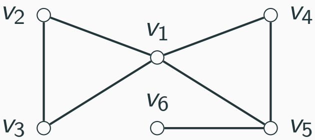

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Next Step: Finding the Fiedler Eigenvalue & Eigenvector.

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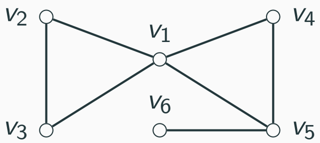

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The Fiedler eigenvalue is about 0.6314.

The Fiedler eigenvector is: $[-0.16, -0.44, -0.44, 0.07, 0.26, 0.71]^T$.

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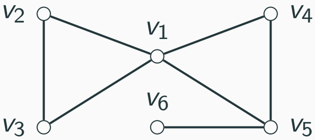

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Final Step: Partition the Vertices.

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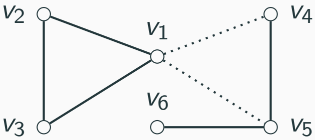

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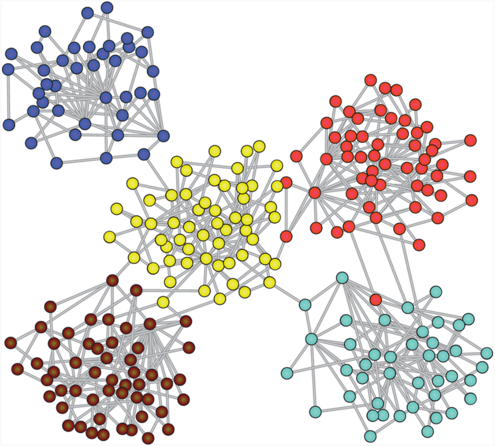
$G_1 = \{v_1, v_2, v_3\}$ while $G_2 = \{v_4, v_5, v_6\}$. The **cut edges** are $v_1 v_4$ and $v_1 v_5$.

Back to the Problem

Detecting Communities: Detects particular groups that are more internally connected. Aids in understanding social structures.

Ex. "People You May Know"...



More Real-World Applications

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Biological Analysis: Spectral partitioning helps analyze complex biological networks, such as gene regulatory networks. It groups genes that are co-regulated or functionally related.