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June 9, 2025

## Spectral Graph Theory and Graph Quantum Mechanics

**Graph Quantum Mechanics**: Intersection of Quantum Mechanics, Linear Algebra, and Graph Theory

Toy Model of Quantum Mechanics: A simplified, discrete model

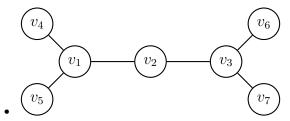
Schrödinger's Equation: Describes the evolution of quantum states

- $\frac{\partial}{\partial t}\Psi = \frac{i}{\hbar}\nabla^2\Psi$
- $\mathbf{F} = \text{ma}$  is the classical analogue to Schrödinger's Equation.

The Schrödinger equation is sensitive to geometry so we can make it discrete

## Discrete Schrodinger Equation:

 $\bullet\,$  Quantum particles live on a graph



In a graph, the Laplacian is a matrix  $\mathbf{E} = \lambda$ 

## Connection to Entropy:

- Entropy: a measure of the disorder of a system
- $S(\rho) = \sum_{i=1}^{n} -\lambda_i \ln \lambda_i \ (\lambda_i \text{ is an eigenvalue of } \rho)$

June 10, 2025

# Intro to Differential Equations and Matrix Exponentials

Origins of differential equations:

- y(t) is function
- $y^1 = 1$

so, 
$$y(t) = t + k$$

(\*Ansatz = a guess)

Method (Integrating Factors):

$$y^{1} = 1$$

$$\frac{dy}{dt} = 1$$

$$dy = dt$$

$$y = \int dt = t + k$$

$$y^{1} = y$$

$$\frac{dy}{dt} = y$$

$$\frac{dy}{y} = dt$$

$$\int \frac{dy}{y} = \int dt$$

$$\ln|y| = t + k$$

$$y = e^{t+k} = e^{k} \cdot e^{t} = ke^{t}$$

Linear systems of Differential Equation:

Step 1: Matrix form:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}^1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

Answer?

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = e^{\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}^t} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

## Matrix Exponential:

- what it is not
- $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$  so  $e^A = \begin{bmatrix} e^1 & e^1 \\ e^1 & e^1 \end{bmatrix}$  THIS IS INCORRECT

Taylor Series: (Taylor expansion on  $e^x$ )

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

$$e^A = I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \frac{A^4}{4!} + \dots$$

$$\begin{array}{cc}
\lambda_1 & 0 \\
0 & \lambda_2
\end{array}$$

$$e^{\begin{bmatrix} \lambda_{1} & 0 \\ 0 & \lambda_{2} \end{bmatrix}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} \lambda_{1} & 0 \\ 0 & \lambda_{2} \end{bmatrix} + \frac{1}{2!} \begin{bmatrix} \lambda_{1}^{2} & 0 \\ 0 & \lambda_{2}^{2} \end{bmatrix} + \frac{1}{3!} \begin{bmatrix} \lambda_{1}^{3} & 0 \\ 0 & \lambda_{2}^{3} \end{bmatrix} + \cdots$$

$$= \begin{bmatrix} \sum_{n=0}^{\infty} \frac{(\lambda_{1})^{n}}{n!} & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{(\lambda_{2})^{n}}{n!} \end{bmatrix} = \begin{bmatrix} e^{\lambda_{1}} & 0 \\ 0 & e^{\lambda_{2}} \end{bmatrix}$$

#### Theorem:

If A is an nxn matrix with eigenvalues  $\lambda_1, \lambda_2, ..., \lambda_n$  then det  $A = (\lambda_1)(\lambda_2)...(\lambda_n)$ 

#### Consequence:

A is non-invertible if one eigenvalue is 0

Theorem 2: If A is matrix that has eigenvalues  $\lambda_1$ )( $\lambda_2$ )...( $\lambda_n$ ), then  $e^A$  has eigenvalues  $e^{\lambda_1}, e^{\lambda_2}, ..., e^{\lambda_n}$ 

June 11, 2025

## Matrix Exponential Proofs and Intro to Graph Theory

## Matrix Exponential Proofs:

## Binomial Theorem:

- Provides a formula for expanding expressions of the form  $(a+b)^n$
- $(x+y)^n = \binom{n}{0}x^n + \binom{n}{1}x^{n-1}y + \binom{n}{2}x^{n-2}y^2 + \dots + \binom{n}{n}y^n$

<u>PF:</u> We know that:

$$e^{At} = I + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \frac{(At)^4}{4!} + \cdots$$

Now we can take the derivative of each term:

$$\frac{d}{dt}e^{At} = 0 + A + \frac{2A^2t}{2!} + \frac{3A^3t^2}{3!} + \frac{4A^4t^3}{4!} + \cdots$$

Simplifying:

$$\frac{d}{dt}e^{At} = A + A^2t + \frac{A^3t^2}{2!} + \frac{A^4t^3}{3!} + \dots = A\left(I + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \dots\right) = Ae^{At}$$

therefore, we conclude : 
$$\frac{d}{dt}(e^{At}) = Ae^{At}$$

## Graph Theory:

- The graph Schrödinger equation connects differential equations + linear algebra + graph theory
- <u>Def</u> A graph is a set (V, E) where V is a set of vertices and E is a set of edges

Non-Directed Graph	Directed Graph
$e = \{v_1, v_2\},  v_1, v_2 \in V$	$e = (v_1, v_2),  v_1, v_2 \in V$
unordered pair	ordered pair (from $v_1$ to $v_2$ )
$v_1$ $v_2$	$v_1$ $v_2$

• <u>Erdös number:</u> describes the "collaborative distance" between mathematician Paul Erdös and another person, as measured by authorship of mathematical papers. (vertices = scholars)

## Combinatorics and Graph Theory Textbook:

#### 1.1

- 1. Digraph (directed graph): each edge of a digraph has a specific orientation
- 2. Multigraph: repeated elements in the set of edges
- 3. Pseudograph: edges connect a vertex to itself
- 4. Hypergraph: edges are arbitrary subsets of vertices
- 5. Infinite graphs: V or E is an infinite set

## 1.2

- V(G): the vertex set of a graph G
- E(G): the edge set
- Order: the cardinality of a graph's vertex set
- Size: the cardinality of a graph's edge set
- Adjacent: given  $v_1, v_2$  if  $v_1, V_2 \in Ethenv_1, v_2$  are adjacent
- If an edge e has a vertex v as an end vertex, v is incident with e
- The neighborhood of a vertex v, denoted by N(v) is the set of vertices adjacent to v
- The First Theorem of Graph Theory: In a graph G, the sum of the degrees of the vertices is equal to twice the number of edges. Consequently, the number of vertices with odd degree is even

#### Perambulation and Connectivity:

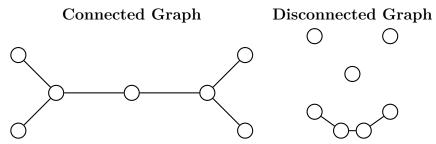
- A <u>walk</u> in a graph is a sequence of (not necessarily distinct) vertices  $v_1, v_2, ..., v_k$  s.t  $v_i v_{i+1} \in E$  for i = 1, 2, ..., k-1. Such a walk is sometimes called a  $v_1 v_k$  walk, and  $v_1$  and  $v_k$  are the end vertices of the walk
- If the vertices in a walk are distinct, then it's called a path
- If the edges in a walk are distinct, then it's called a trail
- Theorem 1.2: In a graph G with vertices  $v_1$  and  $v_2$ , every  $v_1$ - $v_2$  walk contains a  $v_1$ - $v_2$  path
- A graph is connected if every pair of vertices can be joined by a path

June 12, 2025

## **Graph Laplacion**

- $\underline{\mathrm{Def}} \ \Gamma \ (\mathrm{graph}), \ \Gamma = (\mathrm{V}, \ \mathrm{E})$
- deg(V) = number of neighbors
- <u>Def</u> Simple graph: no multi-edges, no loop edges
- <u>Def</u> Connected Components: Maximally Connected Subgraph

## Connected vs. Disconnected Graphs



1 connected component

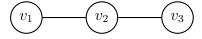
4 connected components

## Degree Matrix

• The degree matrix  $D_{\Gamma}$  of a graph  $\Gamma$  is an  $n \times n$  matrix such that:

$$D_{\Gamma}(i, i) = \deg(v_i)$$
, and  $D_{\Gamma}(i, j) = 0$  for  $i \neq j$ 

• Example:



• The corresponding degree matrix  $D_{\Gamma}$  is:

$$D_{\Gamma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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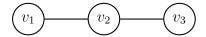
• A disconnected graph will result in a non-invertible matrix

## Adjacency Matrix

• The adjacency matrix  $A_{\Gamma}$  of a graph  $\Gamma$  is an  $n \times n$  matrix where:

$$A_{\Gamma}(i,j) = \begin{cases} 1, & \text{if there is an edge between } v_i \text{ and } v_j \\ 0, & \text{otherwise} \end{cases}$$

- The matrix is symmetric for undirected graphs and has 0s on the diagonal if there are no loops.
- Example:



• The corresponding adjacency matrix  $A_{\Gamma}$  is:

$$A_{\Gamma} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$A_{\Gamma} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Compute the determinant:

$$\det(A_{\Gamma}) = 0$$

Therefore, we conclude that  $A_{\Gamma}$  is not always invertible.

#### The Graph Laplacian

• The graph Laplacian  $\Delta_{\Gamma}$  is defined as:

$$\Delta_{\Gamma} = D_{\Gamma} - A_{\Gamma}$$

PF:

A matrix A is invertible if and only if dim(ker A) = 0. However, for the graph Laplacian  $\Delta_{\Gamma}$ , we know that:

 $\dim(\ker \Delta_{\Gamma}) = \text{number of connected components of } \Gamma$ 

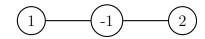
Since this dimension is never zero, it follows that:

$$\dim(\ker \Delta_{\Gamma}) \neq 0$$
,

and therefore we conclude that  $\Delta_{\Gamma}$  is never invertible.

## Graph Quantum Mechanics

• Example:



• Degree matrix:

$$D_{\Gamma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

• Adjacency matrix:

$$A_{\Gamma} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

• Laplacian:

$$\Delta_{\Gamma} = D_{\Gamma} - A_{\Gamma} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

- In a steady state, all vertices within a connected component have the same value.
- The Laplacian helps transfer information across the graph.
- $\ker(\Delta) = \{v \mid \Delta v = 0\} =$ the space of steady states.
- $-\underline{\text{Thm:}} \dim(\ker(\Delta)) = \text{number of connected components (a topological property)}.$

## How about entropy?

$$-Z(\Delta) = -\sum_{i=1}^{n} \lambda_i \ln \lambda_i$$

- $\lambda$  is eiganvalue  $\Delta$
- $-\lambda \neq 0$

June 13, 2025

## Graph Isomorphism, Linear Transformations, and QM

## **Graph Isomorphism**

- <u>Bijection</u>: A function that is both injective (one-to-one) and surjective (onto). A <u>bijection</u> creates a one-to-one correspondence between elements of two sets.
- <u>Linear Transformation</u>: A function  $f: V \to W$  between vector spaces is a linear transformation if:

$$- f(u+v) = f(u) + f(v)$$
$$- f(\lambda u) = \lambda f(u)$$

- A linear transformation is bijective if it is:
  - <u>Injective</u>:  $f(u) = f(v) \Rightarrow u = v$
  - Surjective: Every element in the codomain W has a preimage in the domain V
- $\underline{\mathrm{Def}}\ \Gamma_1 \cong \Gamma_2$  if there exists a bijection  $f: V_1 \to V_2$  such that:

$$\{v, v'\} \in E_1 \iff \{f(v), f(v')\} \in E_2$$

That is,  $\Gamma_1$  and  $\Gamma_2$  have the same structure (same number of vertices and adjacency preserved).

## **Examples of Vector Spaces**

•  $\mathbb{R}$  (dimension = 1)

•  $\mathbb{R}^n$  (dimension = n)

• Matrices of size  $m \times n$  (dimension = mn)

•  $P_d$ : polynomials of degree  $\leq d$  (dimension = d+1)

•  $\mathbb{R}^2 \cong P_1$  (isomorphic since dimensions are equal)

• Isomorphism Theorem:

- If 
$$\dim(V) = \dim(W)$$
, then  $V \cong W$ 

Question: next week: what is the dim of the vector space of quantum vertex states

Answer: dim is  $|v|^n$  (order)

Question: What is the dimension of the space of "steady" states?

Answer:  $\dim(\ker(\Delta))$ 

## Baker-Campbell-Hausdorff Formula

- $e^0 = 1$
- $e^x e^y = e^{x+y}$
- $e^A e^B \neq e^{A+B}$
- Baker–Campbell–Hausdorff Formula:  $e^A e^B = e^{A+B+...}$
- ... = f([A, B)] = AB BA, the commutator

## In Quantum Mechanics

- Matrix A represents an observable (i.e., a measurable quantity).
- Examples: position, momentum, energy, entropy
- Heisenberg's Uncertainty Principle:
  - In classical mechanics, position and momentum can be known with absolute precision.
  - In quantum mechanics, there is a limit to how precisely both can be known simultaneously.

## Regular Graph

• All vertices have same degree

#### **Entropy Notes**

## What is Entropy?

- Entropy quantifies uncertainty or lack of information about a system.
- It is observer-dependent and not an intrinsic property.
- The Second Law of Thermodynamics: entropy increases over time.
- Entropy explains the direction of time and large-scale predictability.

## Historical Background

- Carnot (1824): Not all heat is convertible to work.
- Clausius: Coined *entropy*, stated it trends toward a maximum.
- Boltzmann: Defined entropy via the number of microstates per macrostate.

#### Statistical View

- High entropy implies many possible microstates.
- Natural progression: low to high entropy (more probable states).
- Defines the thermodynamic arrow of time.

#### Information Theory

- Shannon defined entropy as message unpredictability.
- Structural similarity between Shannon and Boltzmann entropy.
- High entropy: patternless; low entropy: structured.
- "Entropy is what we don't know; information is what we do." Seth Lloyd

#### Modern Interpretations

- Gibbs: Entropy increases with particle mixing.
- Von Neumann: Tracks quantum state uncertainty.
- Bekenstein-Hawking: Connects entropy to black hole event horizons.

#### Subjectivity in Entropy

- Observer perspective affects entropy values (Gibbs paradox).
- "Observational entropy" integrates measurable information.

#### **Entropy and Computation**

- Perfect knowledge: entropy is constant, time doesn't flow.
- Coarse-graining due to limited computation explains perceived time.

#### **Applications**

- Machine learning: Entropy used in compression algorithms.
- Physics: Szilard's engine converts information into physical work.

## Von Neumann Entropy of Graphs

- Measures structural complexity via spectral properties.
- Laplacian and normalized Laplacian versions.
- Higher entropy: more components, longer paths, greater symmetry.

## Applications

• Network analysis, graph classification, and centrality metrics.

## **Approximations and Limitations**

- Quadratic approximation based on degree distribution.
- Less accurate for irregular or complex networks.

## Interpretation

- Captures randomness and structure in network form.
- Bridges thermodynamics, quantum mechanics, and information theory.

June 16, 2025

## Types of Graphs

<u>Thm</u> Eiganvalues of  $(\Delta)$  are non-negative (week long HW)

## Types of Graphs

- 1. Complete Graphs: A complete graph of order n is denoted by  $K_n$ .
- 2. Empty Graphs: The empty graph on n vertices, denoted by  $E_n$ , is the graph of order n where E is the empty set.
- 3. Complements: Given a graph G, the *complement* of G, denoted by  $\overline{G}$ , is the graph whose vertex set is the same as that of G, and whose edge set consists of all the edges that are not present in G.
- 4. Regular Graphs: A graph G is regular if every vertex has the same degree. G is regular of degree r (i.e., r-regular) if deg(v) = r for all vertices v in G. Complete graphs of order n are regular of degree n-1, and empty graphs are regular of degree 0.
- 5. Cycles: The graph  $C_n$  is a cycle on n vertices.
- 6. Paths: The graph  $P_n$  is a path on n vertices.
- 7. Subgraphs: A graph H is a subgraph of a graph G if  $V(H) \subset V(G)$  and  $E(H) \subset E(G)$ .
- 8. Induced Subgraphs: Given a graph G and a subset S of the vertex set, the subgraph of G induced by S, denoted  $\langle S \rangle$ , is the subgraph with vertex set S and edge set  $\{uv \mid u, v \in S \text{ and } uv \in E(G)\}$ . So,  $\langle S \rangle$  contains all the vertices of S and all edges of G whose end vertices are both in S.
- 9. Bipartite Graphs: A graph G is bipartite if its vertex set can be partitioned into two sets X and Y in such a way that every edge of G has one end vertex in X and the other in Y. In this case, X and Y are called the *partite sets*. A bipartite graph with partite sets X and Y is called a complete bipartite graph if its edge set is of the form  $E = \{xy \mid x \in X, y \in Y\}$  (that is, if every possible connection of a vertex in X with a vertex in Y is present). Such a graph is denoted by  $K_{|X|,|Y|}$ .

- 10. Tree Graphs: Connected graph with no cycles
- 11. Star Graphs: A tree with exactly one vertex of degree greater than 1 (the central vertex) and all other vertices having degree 1 (leaf vertices)

June 17, 2025

## Incidence Matrix and Odd Laplacian

Incidence Matrix: Let  $\Gamma$  be a directed graph with |V| = n vertices and |E| = m edges. The incidence matrix  $I_{\Gamma}$  is an  $n \times m$  matrix defined as follows:

$$I(i,j) = \begin{cases} -1 & \text{if edge } e_j \text{ starts at vertex } v_i, \\ 1 & \text{if edge } e_j \text{ ends at vertex } v_i, \\ 0 & \text{otherwise.} \end{cases}$$

**Example:** For the directed path  $v_1 \to v_2 \to v_3$ , the incidence matrix  $I_{\Gamma}$  is:

$$I_{\Gamma} = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$$

The transpose of the incidence matrix  $I_{\Gamma}$  is:

$$I_{\Gamma}^{\top} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$

 $I_{\Gamma}^{\top}I_{\Gamma}$  (the **odd Laplacian**):

$$I_{\Gamma}^{\top}I_{\Gamma} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

 $I_{\Gamma}I_{\Gamma}^{\top}$  (the even Laplacian):

$$I_{\Gamma}I_{\Gamma}^{\top} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

The graph Laplacian is defined as

$$\Delta_{\Gamma} = D_{\Gamma} - A_{\Gamma}$$

$$D_{\Gamma} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad A_{\Gamma} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

$$\Delta_{\Gamma} = D_{\Gamma} - A_{\Gamma} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}.$$

 $\underline{\text{Theorem}} \quad \Delta = II^{\top}$ 

•  $\Delta_+$  (even):  $D - A = II^{\top}$ 

•  $\Delta_{-}$  (odd):  $I^{\top}I$ 

## Fermions and Bosons

• Superlaplacian:

$$\Delta = \begin{pmatrix} \Delta_+ & 0 \\ 0 & \Delta_- \end{pmatrix}$$

• Observation:  $\Delta_+$  and  $\Delta_-$  have the same non-zero eigenvalues.

• dim  $\ker(\Delta_+)$  = number of zero eigenvalues = number of connected components =  $b_0$ .

• dim ker( $\Delta_{-}$ ) = number of independent cycles =  $b_1$ .

• Theorem:

 $b_0 - b_1 = |V| - |E| \rightarrow \text{topological invariant.}$ 

June 18, 2025

# Entropy/Gluing, and the Weighted Laplacian

Observation: If  $\Gamma_1 \cong \Gamma_2$ , then  $S(\Delta_{\Gamma_1}) = S(\Delta_{\Gamma_2})$ .

<u>Def</u> Two graphs  $\Gamma_1$  and  $\Gamma_2$  are iso-entropic if  $S(\Gamma_1) = S(\Gamma_2)$ .

<u>Def</u> Two graphs are isospectral if they have the same eigenvalues.

## **Overarching Questions**

Q: Von Neumann Entropy and Gluing

- Let  $\Gamma_1$  and  $\Gamma_2$  be graphs, and consider the following types of gluing:
  - $-\Gamma_1 \cup \Gamma_2$  (interface gluing)
  - $\Gamma_1 \cup \Gamma_2$  (bridge gluing)
  - $\underline{\operatorname{Conj.}} S(\Gamma_1 \cup \Gamma_2) \ge S(\Gamma_1) + S(\Gamma_2)$

 $\underline{\mathrm{Def:}}$  Interface Gluing: glue on isomorphic subgraphs

Ex.



Ex. Pair of pants decomposition

<u>Def:</u> Bridge Gluing

Ex.



Cheeger Inequalities: Measurements of bottlenecks

**Disjoint Union:**  $\Gamma_1 \cup \Gamma_2$  — place them near each other

•  $S(\Gamma_1 \cup \Gamma_2) = S(\Gamma_1) + S(\Gamma_2)$ 

## Weighted Laplacian:

- Normalized Laplacian:  $\Delta_N = D^{1/2} \Delta D^{-1/2}$
- Weights:

$$A_w(i,j) = \begin{cases} w_{ij}, & \text{if } v_i v_j \in E \\ 0, & \text{otherwise} \end{cases}$$

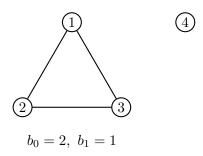
$$v_1$$
  $v_2$   $v_3$ 

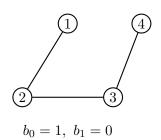
The weighted adjacency matrix  $A_w$  is:

$$A_w = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}$$

June 20, 2025

# Rewiring/Gluing of the Laplacian and their Spectra Rewiring:





• 
$$b_0 - b_1 = 1$$
 for both

 $\underline{\mathbf{Q}}$  What is rewiring in higher dimensions?

## Gluing Formulas for the Laplacian:

• Bridge Gluing:  $\Delta_{\Gamma_1}^{+1} \cup_B \Delta_{\Gamma_2}^{+1} = \begin{pmatrix} \Delta_{\Gamma_1}^{+1} & 0 \\ 0 & \Delta_{\Gamma_2}^{+1} \end{pmatrix}$ 

## Gluing of Graph Laplacians and their Spectra Summary:

## The paper studies a central question in spectral graph theory:

How do the Laplacians, and their spectra behave when two graphs are glued?

The paper addresses this by introducing and analyzing two ways of gluing graphs:

- Interface gluing
- Bridge gluing

The paper then derives how these operations affect the even and odd graph Laplacians and their spectra, and discuss applications in quantum mechanics and network theory.

## Gluing Methods:

Interface Gluing In interface gluing, two graphs are joined by identifying a common subgraph. This subgraph is called the interface. The result is that the two graphs share this overlapping structure in the glued graph.

**Bridge Gluing** In contrast, bridge gluing begins with two graphs, and then introduces a new edge that connects selected vertices from each graph. This is structurally different: instead of merging shared parts, it preserves the original graphs intact and simply connects them.

## Even and Odd Graph Laplacians

Even Laplacian ( $\Delta^+$ ) Acts on functions defined on vertices. Measures how much a function at a vertex differs from values at its neighboring vertices. Defined as:  $\Delta^+ = II^T$ , where I is the incidence matrix of the graph. Independent of edge orientation. Discrete analog of the Laplacian operator in  $\mathbb{R}^n$ .

Odd Laplacian ( $\Delta^-$ ) Acts on functions defined on edges. Measures how values assigned to edges vary along incident edges. Defined as:  $\Delta^- = I^T I$  Depends on edge orientation.

**Key Insight:** Although  $\Delta^+$  and  $\Delta^-$  act on different spaces and depend differently on orientation, the authors prove that they are isospectral, meaning that they have the same nonzero eigenvalues with the same multiplicities, even though their kernels differ. This is super important as it allows us to analyze one Laplacian and recover spectral information that is still true about the other.

#### Spectral Effects of Gluing

#### Matrix Formulations

For both gluing types, the authors derive explicit matrix formulas for the Laplacians of the resulting graphs.

Interface gluing: The Laplacians are formed by merging the matrices along the shared subgraph, treating overlapping vertices and edges as one. The diagonal entries (degrees) are updated to reflect connections from both graphs, while off-diagonal entries capture any new adjacencies introduced by the gluing.

Bridge gluing: The new Laplacian becomes a block matrix. It includes the original Laplacians plus correction terms corresponding to the added bridge edges.

Spectral Relationships To make this practical, the authors prove relationships be-

tween characteristic polynomials:

For interface gluing of graphs  $\Gamma_1$  and  $\Gamma_2$  along interface I:

$$E(\Gamma_1 \sqcup_I \Gamma_2) = \frac{E(\Gamma_1)E(\Gamma_2)}{E(I)}$$

For bridge gluing with bridge graph B:

$$E(\Gamma_1 \sqcup_B \Gamma_2) = \frac{E(\Gamma_1)E(\Gamma_2)}{E(B)}$$

Here,  $E(\Gamma)$  is the characteristic polynomial of the even Laplacian

#### Why does this matter?

It means we can compute the spectrum of a complex graph from the spectra of its parts, with correction terms that depend only on the interface or bridge. This avoids recomputing everything from scratch.

## The Fiedler Value (Algebraic Connectivity)

*Def:* The Fiedler value is the smallest nonzero eigenvalue of the even Laplacian. It describes how well-connected the graph is.

However, computing the Fiedler value directly is hard, especially for large graphs.

So, the paper gives an algorithm that computes or estimates the Fiedler value of a glued graph using:

- The spectra of the components
- The structure of the bridge or interface

## **Quantum Mechanics**

In discrete quantum mechanics, the graph Laplacian acts like the Hamiltonian in the Schrödinger equation:

$$\Delta_{\Gamma}\Psi = E\Psi$$

where:

- $\Psi$  is a wavefunction defined on the graph's vertices,
- E is the energy,
- the eigenvalues of  $\Delta_{\Gamma}$  represent the energy levels.

Using gluing, the paper shows how to build composite quantum systems from smaller ones. This allows:

- computing partition functions
- implementing a combinatorial version of the Feynman path integral, which is a way to sum over quantum paths on a graph.

A key result is that eigenvectors of the glued graph behave predictably, which makes it efficient to compute time evolution in large quantum systems.

## **Applications**

#### **Quantum Mechanics**

In discrete quantum mechanics, the graph Laplacian acts like the Hamiltonian (which represents kinetic energy) in the Schrödinger equation:

$$\Delta_{\Gamma}\Psi = E\Psi$$

where:  $\Psi$  is a wavefunction defined on the graph's vertices, E is the energy, and the eigenvalues of  $\Delta_{\Gamma}$  represent the energy levels.

Using gluing, the paper shows how to build composite quantum systems from smaller ones. This allows:

- computing partition functions
- implementing a combinatorial version of the Feynman path integral

A key result is that eigenvectors of the glued graph behave predictably, which makes it efficient to compute time evolution in large quantum systems.

The paper also proposes a modular electronic structure model. This approach enables parallel computation of quantum properties.

Finally, inspired by Witten's ideas in supersymmetry, they connect spectral properties of the graph (like eigenvalues) to topological features such as the Euler characteristic and Betti numbers.

#### Network Theory and Bottleneck Detection

In network science, the eigenvalues of the graph Laplacian provide important information about:

- Connectivity (via the Fiedler value)
- Bottlenecks (via the Cheeger constant)

The paper shows that gluing operations affect these spectral quantities in predictable ways

The authors also extend their results to the normalized Laplacian. This extension is especially useful when analyzing real-world graphs

June 23, 2025

# Euler Characteristic, Diagonalization

**Euler Characteristic:** 

$$\underline{\mathrm{Def}} \quad \chi(\Gamma) = |V| - |E|$$

$$\underline{\text{Thm}} \quad \chi(\Gamma) = b_0 - b_1$$

What is  $\chi$  for gluing?

Bridge:

Ex.



- $\chi(\Gamma_1) = 1$
- $\chi(\Gamma_2) = 1$
- $\chi(B) = 1$
- $\chi(\Gamma_1 \cup \Gamma_2) = 1$

$$\underline{\text{Thm}} \quad \chi(\Gamma_1 \cup \Gamma_2) = \chi(\Gamma_1) + \chi(\Gamma_2) - \chi(B)$$

So, 
$$\frac{E(\Gamma_1) \cdot E(\Gamma_2)}{E(B)}$$

## Diagonalization:

Let M be a matrix with eigenvalues.

We say M is diagonalizable if there exists a matrix Q such that

$$D = Q^{-1}MQ$$

If so, Q is a matrix whose columns are eigenvectors of M, and D is a diagonal matrix whose diagonal entries are the corresponding eigenvalues.

## Applications:

$$D^{n} = Q^{-1}M^{n}Q$$
 
$$D^{2} = (Q^{-1}MQ)(Q^{-1}MQ) = Q^{-1}M^{2}Q$$
 
$$M^{2025} = QD^{2025}Q^{-1}$$

<u>Thm:</u> M is diagonalizable if and only if, for every eigenvalue  $\lambda$ ,

algebraic multiplicity( $\lambda$ ) = geometric multiplicity( $\lambda$ )

This condition must hold for *all* eigenvalues of M.

## What if M is not diagonalizable?

- M can be approximated by diagonalizable matrices.
- That is, there exists a sequence  $\{M_k\}$  of diagonalizable matrices such that  $M_k \to M$ .

June 25, 2025

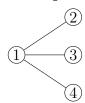
## **Small World Networks**

Characteristic Path Length:

• Definition:

$$L_{\Gamma} = \frac{\sum d(v, w)}{\binom{n}{2}}$$

• Example:



$$L_{\Gamma} = \frac{1+1+2+2+2}{6} = \frac{9}{6} = \frac{3}{2}$$

• In general,  $P_n$  (the path graph) has the largest characteristic path length

<u>Def:</u> For  $v \in V$ , the clustering coefficient is:

$$cc(v) = \frac{|E(\langle N[v] \rangle)|}{|E(K_{\deg(v)+1})|}$$

Average clustering coefficient:

$$cc(\Gamma) = \frac{\sum_{v \in V} cc(v)}{n}$$

<u>Def:</u> A small world network is a sparse graph such that:

- $L(\Gamma)$  is small
- $cc(\Gamma)$  is large

Question: In what way does a small world network relate to entropy? \*Is this the idea?\*

High clustering  $\Rightarrow$  low entropy, Short characteristic path length  $\Rightarrow$  high entropy

## 1.2.3 in Graph Theory Book:

**Acquaintance Graph:** A graph where each vertex represents a person, and an edge connects two vertices if the corresponding people know each other.  $\rightarrow$  *Is this graph connected?* Potentially. However, if the graph is disconnected, there is one very large connected component.

**Six Degrees Theory:** Asserts that, given any pair of individuals, there exists a chain of no more than six acquaintance connections joining them.

#### Small-World Network: What makes a small world small?

- 1. Plenty of mutual acquaintances
- 2. The graph should be sparse in edges
- 3. Distances between pairs of vertices should be relatively small
- 4. There should be a reasonable amount of clustering
- 5. Low characteristic path lengths and high clustering coefficients

## **SWN** Readings:

Many systems, such as the internet, social groups, and biochemical pathways, have been described as exhibiting small-world properties, characterized by high clustering and short path lengths. This paper critiques the widely used small-world coefficient  $\sigma$ , defined as:

$$\sigma = \frac{C/C_{\text{rand}}}{L/L_{\text{rand}}}$$

where C is the clustering coefficient, L is the characteristic path length, and  $C_{\text{rand}}$ ,  $L_{\text{rand}}$  are the corresponding values from an equivalent random network.

#### Limitations of $\sigma$ :

- Overestimates small-worldness: even networks with low absolute clustering can be labeled small-world if  $C_{\text{rand}}$  is very low.
- Highly sensitive to small fluctuations in  $C_{\text{rand}}$ .
- Depends on network size;  $\sigma$  tends to increase in larger networks.
- Cannot distinguish where a network lies on the lattice–random spectrum.

## Solution: The $\omega$ Index

To resolve these issues, the authors define a new small-world measure:

$$\omega = \frac{L_{\rm rand}}{L} - \frac{C}{C_{\rm latt}}$$

where  $C_{\text{latt}}$  is the clustering of an equivalent lattice network. This formulation better reflects the original intuition of Watts and Strogatz.

## Properties of $\omega$ :

- Values are bounded between -1 and 1.
- $\omega \approx 0$ : Network has small-world properties (high clustering and short path length).
- $\omega < 0$ : More lattice-like (longer path length, high clustering).
- $\omega > 0$ : More random-like (short path length, low clustering).
- Network-size invariant: more consistent across different scales.

## Interpretation:

- A typical small-world range is approximately  $-0.5 \le \omega \le 0.5$ .
- $\omega$  enables continuous comparison and positioning of a network along the lattice / small-world / random spectrum.

July 1, 2025

# Topology v. Entropy

## Topology

- Graph topology
- 1-dimensional object (vertices + edges)
- $b_0$ : number of connected components
- $b_1$ : number of independent cycles
- $\Delta_+$ ,  $\Delta_-$  knows about topology
- $\dim(\ker(\Delta_+)) = b_0$
- $\dim(\ker(\Delta_-)) = b_1$

## Entropy

- $\Delta_+$ ,  $\Delta_-$  knows about entropy
- Entropy: "non-topological info"

July 2, 2025

## Quick Intro to Morse Theory

## Morse Theory

- Continuum  $\rightarrow$  Discrete
- Goal of Morse Theory: Study topological invariants using multivariable calculus.
- Index = number of downward directions at a critical point

## Morse Theorem:

$$C_0 - C_1 + C_2 = \chi$$

#### where:

- $C_0$  = number of critical points of index 0
- $C_1$  = number of critical points of index 1
- $C_2$  = number of critical points of index 2
- $\chi$  is the Euler characteristic.

When you "punch" a torus to deform it, the number of critical points may change, but the Euler characteristic  $\chi$  remains unchanged.

July 3, 2025

## Graph Theory Notes for Project

## **Distance Matrix**

Let D(i, j) be the distance between vertex  $v_i$  and vertex  $v_j$  in a graph. The distance matrix records all such distances.

- symmetric
- 0 in diagonal

## **Eccentricity:**

The eccentricity ecc(v) of a vertex v is the greatest distance between v and any other vertex in the graph:

$$\mathrm{ecc}(v) = \max_{x \in V} d(v, x)$$

## Radius of a Graph:

The radius of a graph G is the smallest eccentricity among all vertices:

$$\mathrm{rad}(G) = \min_{v \in V} \mathrm{ecc}(v)$$

## Diameter of a Graph:

The diameter of a graph G is the largest eccentricity among all vertices:

$$\operatorname{diam}(G) = \max_{v \in V} \operatorname{ecc}(v)$$

Inequality:

$$rad(G) \le diam(G) \le 2 \cdot rad(G)$$

## Center of a Graph:

The center C of a graph is the set of all vertices whose eccentricity equals the radius:

$$C = \{v \in V \mid \mathrm{ecc}(v) = \mathrm{rad}(G)\}$$

## Periphery of a Graph:

The periphery of a graph is the set of vertices whose eccentricity equals the diameter:

$$\operatorname{Periphery}(G) = \{v \in V \mid \operatorname{ecc}(v) = \operatorname{diam}(G)\}$$

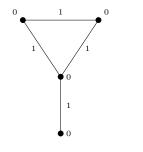
July 7, 2025

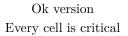
# Discrete Morse Theory

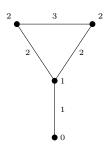
In the continuum Morse theory is:

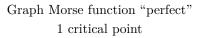
$$C_0 - C_1 + C_2 = b_0 - b_1 + b_2 = \chi(M)$$

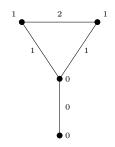
In discrete Morse theory on graphs, the Morse function changes value at least once if there is a change in dimension, reflecting topology changes.











Not Morse

On a graph, the Euler characteristic is:

$$C_0 - C_1 = b_0 - b_1 = |V| - |E|.$$

Morse Inequality for graphs:

- $b_0 \le C_0$
- $b_1 \le C_1$

# Homework Questions

## HW1: What are the steady states?

**Answer:** Steady states are functions that do not change over time. These include constant functions or any functions for which the Laplacian (or second derivative) is zero.

<u>PF:</u> For a function  $\Psi$  to remain unchanged over time, its second derivative must vanish:

$$\nabla^2 \Psi = 0$$

## HW2: Solve

(a) 
$$y' = 5y$$

$$ln |y| = 5t + k$$

$$y = e^{5t+k} = ke^{5t}$$

(b) 
$$y' = -y + 1$$

$$y' = -y + 1$$

$$\frac{dy}{dt} = -y + 1$$

$$\int \frac{dy}{1 - y} = \int dt$$

$$-\ln|1 - y| = t + k$$

$$\ln|1 - y| = -t - k$$

$$1 - y = e^{-t - k} = -ke^{-t}$$

$$y = 1 + ke^{-t}$$

## HW3: Matrix exponentials

(a) 
$$e^{\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}}$$

$$e^{\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}} = \sum_{n=0}^{\infty} \frac{1}{n!} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}^n = \begin{bmatrix} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{1}{n!} \end{bmatrix} = \begin{bmatrix} e^{-1} & 0 \\ 0 & e \end{bmatrix}$$

(b) 
$$e^{\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}}$$

$$e^{\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}} = \sum_{n=0}^{\infty} \frac{1}{n!} \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}^n$$

$$= \begin{bmatrix} \sum_{n=0}^{\infty} \frac{(\lambda_1)^n}{n!} & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{(\lambda_2)^n}{n!} \end{bmatrix} = \begin{bmatrix} e^{\lambda_1} & 0 \\ 0 & e^{\lambda_2} \end{bmatrix}$$

**HW4:** Let A be any square matrix. Prove that  $e^A$  is always invertible.

We want to show that  $e^A e^{-A} = I$ , where

$$e^{A} = \sum \frac{A^{m}}{m!},$$
$$e^{-A} = \sum \frac{(-A)^{n}}{n!}.$$

We multiply the two series:

$$e^A e^{-A} = \left(\sum \frac{A^m}{m!}\right) \left(\sum \frac{(-A)^n}{n!}\right).$$

This gives another power series:

$$e^A e^{-A} = \sum$$
 (some coefficient)  $\cdot A^k$ .

Now we solve for the coefficient of  $A^k$ . We get:

$$\left(\frac{1}{k!} + \frac{(-1)^k}{k!}\right) + \left(\frac{-1}{(k-1)! \cdot 1!} + \frac{(-1)^{k-1}}{(k-1)! \cdot 1!}\right) + \left(\frac{-1}{(k-2)! \cdot 2!} + \frac{(-1)^{k-2}}{(k-2)! \cdot 2!}\right) + \dots$$

We observe two cases:

- 1. k is odd, the terms alternate and cancel in pairs.
- 2. k is even, we can factor and rewrite the full sum as:

$$\frac{1}{k!} \sum_{l=0}^{k} (-1)^l \binom{k}{l},$$

where

$$\binom{k}{l} = \frac{k!}{(k-l)! \cdot l!}.$$

By the binomial identity:

$$\sum_{l=0}^{k} (-1)^{l} \binom{k}{l} = \begin{cases} 1 & \text{if } k = 0, \\ 0 & \text{if } k > 0. \end{cases}$$

Therefore, the coefficient is 1 when k = 0 and 0 for all k > 0, so:

$$e^A e^{-A} = I.$$

This also means  $e^{-A}e^A=I$ , so  $e^A$  has an inverse. We conclude that

$$(e^A)^{-1} = e^{-A},$$

so  $e^A$  is always invertible.

**HW5:** Verify that  $\frac{d}{dt}(e^{At}) = Ae^{At}$ .

PF: We know that:

$$e^{At} = I + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \frac{(At)^4}{4!} + \cdots$$

Now we can take the derivative of each term:

$$\frac{d}{dt}e^{At} = 0 + A + \frac{2A^2t}{2!} + \frac{3A^3t^2}{3!} + \frac{4A^4t^3}{4!} + \cdots$$

Simplifying:

$$\frac{d}{dt}e^{At} = A + A^2t + \frac{A^3t^2}{2!} + \frac{A^4t^3}{3!} + \dots = A\left(I + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \dots\right) = Ae^{At}$$

therefore, we conclude : 
$$\frac{d}{dt}(e^{At}) = Ae^{At}$$

**HW6:** Is  $A_{\Gamma}$  always invertible?

$$A_{\Gamma} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \Rightarrow \quad \det(A_{\Gamma}) = 0$$

So  $A_{\Gamma}$  is not always invertible.

**HW7:** Prove that  $\Delta_{\Gamma}$  is never invertible.

<u>PF</u>: A matrix A is invertible if and only if dim(ker A) = 0. For the graph Laplacian  $\Delta_{\Gamma}$ ,

 $\dim(\ker \Delta_{\Gamma}) = \text{number of connected components of } \Gamma$ 

This is always at least 1, so  $\Delta_{\Gamma}$  is never invertible.

**HW8:** Prove or disprove: If a graph is regular, the adjacency matrix is always invertible.

## PF:

I will disprove this statement by providing a counterexample. Consider the regular graph  $C_4$ . Its adjacency matrix A is:

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

Calculating the determinant, we find det(A) = 0. Since the determinant is zero, the matrix A is not invertible.

Therefore, we conclude that the adjacency matrix of a regular graph is not always invertible.

**HW9:** Compute  $S(\Delta_{\Gamma})$  for the path graph on three vertices.

The Laplacian matrix of the path graph on three vertices is:

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

We compute the characteristic polynomial:

$$\det(\Delta_{\Gamma} - \lambda I) = (-\lambda)(\lambda - 1)(\lambda - 3)$$

So, the eigenvalues are:

$$\lambda_1 = 0, \quad \lambda_2 = 1, \quad \lambda_3 = 3$$

Now:

$$\sum \lambda \ln \lambda = 1 \cdot \ln 1 + 3 \cdot \ln 3 = 0 + 3 \ln 3 = 3 \ln 3 \approx 3.30$$

**HW10:** Prove that  $det(A) = \lambda_1 \lambda_2 \lambda_3$ .

<u>PF:</u>

Let A be a  $3 \times 3$  matrix with eigenvalues  $\lambda_1, \lambda_2, \lambda_3$ .

The eigenvalues of A are the roots of its characteristic polynomial:

$$\chi_A(\lambda) = \det(A - \lambda I).$$

This characteristic polynomial can be factored as:

$$\chi_A(\lambda) = -(\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3).$$

Evaluating at  $\lambda = 0$ :

$$\chi_A(0) = -(0 - \lambda_1)(0 - \lambda_2)(0 - \lambda_3) = -(-\lambda_1)(-\lambda_2)(-\lambda_3) = -(-1)\lambda_1\lambda_2\lambda_3 = \lambda_1\lambda_2\lambda_3.$$

Since  $\chi_A(0) = \det(A)$ , we conclude:

$$\det(A) = \lambda_1 \lambda_2 \lambda_3.$$

**HW11:** Prove that if A has eigenvalues  $\lambda_1, \lambda_2, \lambda_3$ , then  $e^A$  has eigenvalues  $e^{\lambda_1}, e^{\lambda_2}, e^{\lambda_3}$ .

<u>PF:</u>

Let A have eigenvalues  $\lambda_1, \lambda_2, \lambda_3$ . Suppose that A is diagonalizable. That is, there exists a matrix Q such that

$$A = Q^{-1}DQ$$

where D is a diagonal matrix with the eigenvalues of A on the diagonal.

Now consider the matrix exponential:

$$e^{A} = I + A + \frac{A^{2}}{2!} + \frac{A^{3}}{3!} + \dots + \frac{A^{k}}{k!}$$

Substituting  $A = Q^{-1}DQ$ , we get:

$$e^{A} = I + Q^{-1}DQ + \frac{(Q^{-1}DQ)^{2}}{2!} + \frac{(Q^{-1}DQ)^{3}}{3!} + \dots + \frac{(Q^{-1}DQ)^{k}}{k!}$$

Using the fact that  $(Q^{-1}DQ)^k = Q^{-1}D^kQ$  and that matrix multiplication is associative, we simplify:

$$e^{A} = \sum_{k=0}^{\infty} \frac{(Q^{-1}DQ)^{k}}{k!} = \sum_{k=0}^{\infty} \frac{Q^{-1}D^{k}Q}{k!} = Q^{-1} \left(\sum_{k=0}^{\infty} \frac{D^{k}}{k!}\right) Q = Q^{-1}e^{D}Q$$

Now, since  $D = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$ , we know that

$$e^D = \operatorname{diag}(e^{\lambda_1}, e^{\lambda_2}, e^{\lambda_3})$$

Thus, we conclude that  $e^A$  is diagonalizable and has eigenvalues  $e^{\lambda_1}, e^{\lambda_2}, e^{\lambda_3}$ .

HW12: Show that the following graphs are isomorphic to each other:

•  $K_{2,2} \cong C_4$ : Both graphs have 4 vertices, and each vertex has degree 2. The graph  $K_{2,2}$  is bipartite with vertex sets  $X = \{x_1, x_2\}$  and  $Y = \{y_1, y_2\}$ , and edges connecting every vertex in X to every vertex in Y. The cycle graph  $C_4$  has vertices  $v_1, v_2, v_3, v_4$  connected in a cycle.

We can define a bijection:

$$f: V(K_{2,2}) \to V(C_4), \quad f(x_1) = v_1, \quad f(y_1) = v_2, \quad f(x_2) = v_3, \quad f(y_2) = v_4.$$

Observe that adjacency is preserved: In  $K_{2,2}$ , edges are exactly between vertices in X and Y, and under f, these map to edges between adjacent vertices in  $C_4$ . Therefore,

$$(x,y) \in E(K_{2,2}) \iff (f(x), f(y)) \in E(C_4).$$

Thus, we conclude that  $K_{2,2}$  and  $C_4$  are isomorphic.

•  $K_2 \cong P_2$ : Both graphs have two vertices connected by a single edge. We can label vertices as  $v_1, v_2$  in both graphs. Observe that the identity map

$$f: V(K_2) \rightarrow V(P_2), \quad f(v_i) = v_i$$

preserves adjacency, since

$$(v_1, v_2) \in E(K_2) \iff (f(v_1), f(v_2)) \in E(P_2).$$

Thus, we conclude  $K_2$  and  $P_2$  are isomorphic.

**HW13:** Consider the cycle graph  $C_3$  with vertices labeled  $v_1, v_2, v_3$ .

1. The edges of  $C_3$  are oriented clockwise:

$$v_1 \rightarrow v_2, \quad v_2 \rightarrow v_3, \quad v_3 \rightarrow v_1.$$

Compute the odd Laplacian  $\Delta_{-}$  of this graph, and determine  $\dim(\ker(\Delta_{-}))$ .

• The incidence matrix is:

$$I = \begin{bmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$$

• The odd Laplacian is:

$$\Delta_{-} = (I)^{\top} I = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

• Since the number of independent cycles is one:

$$\dim(\ker(\Delta_{-})) = 1$$

2. Now modify the graph by reversing the direction of one edge, so that the edge from  $v_2$  to  $v_3$  is instead  $v_3 \rightarrow v_2$ :

$$v_1 \rightarrow v_2, \quad v_3 \rightarrow v_2, \quad v_3 \rightarrow v_1.$$

Again compute the odd Laplacian  $\Delta_{-}$  for this modified graph, and determine dim(ker( $\Delta_{-}$ )).

• The incidence matrix is:

$$I = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & -1 & -1 \end{bmatrix}$$

• The odd Laplacian is:

$$\Delta_{-} = I^{\top} I = \begin{bmatrix} 2 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 2 \end{bmatrix}$$

• Since the graph is no longer a cycle:

$$\dim(\ker(\Delta_{-})) = 0$$

Follow up question: What happens with  $\Delta_{-}$  when we change directions?

• The eigenvalues are preserved. ADD MORE

**HW16:** Compute the characteristic polynomial for complete graph  $K_n$ .

$$\Delta(K_n) = \begin{pmatrix} n-1 & -1 & -1 & -1 & \cdots \\ -1 & n-1 & -1 & -1 & \cdots \\ -1 & -1 & n-1 & -1 & \cdots \\ -1 & -1 & -1 & n-1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

We want to find the eigenvalues of the Laplacian matrix  $\Delta$  of the graph  $K_n$ . Since  $K_n$  is connected, we know that  $\Delta$  has eigenvalue 0 with multiplicity 1. Now, we know  $\Delta$  has eigenvalue n, so we consider

$$\dim(\ker(\Delta - nI)).$$

Note that

$$\Delta - nI = M$$
,

where M is the  $n \times n$  matrix of all negative ones.

Therefore,

$$\ker(\Delta - nI) = \ker(M).$$

When we row-reduce the matrix M, we observe that it has only one pivot column. Using the Rank-Nullity Theorem,

$$n = \operatorname{rank}(M) + \dim(\ker(M)) \implies \dim(\ker(M)) = n - 1.$$

Thus, the eigenvalue n has multiplicity n-1.

We conclude that the characteristic polynomial of  $\Delta$  is

$$P_{\Delta_{K_n}}(\lambda) = \lambda(\lambda - n)^{n-1}.$$

**HW17:** If  $\Gamma$  is regular of degree d, find an explicit relationship between  $S(\Delta)$ , S(A), and d.

Since  $\lambda$  is an eigenvalue of A, there exists a vector v such that:

$$Av = \lambda v$$
.

Multiplying both sides by -1:

$$-Av = -\lambda v$$
.

Now consider:

$$(dI)v - Av = (dI)v - \lambda v,$$

which gives

$$(dI - A)v = dv - \lambda v$$
,

and thus

$$(dI - A)v = (d - \lambda)v.$$

Therefore,  $(d - \lambda)$  is an eigenvalue of  $\Delta = dI - A$ .

Now, we can compare the entropies:

$$S(A) = \sum_{i} \lambda_{i} \ln \lambda_{i},$$
  
$$S(\Delta) = \sum_{i} (d - \lambda_{i}) \ln(d - \lambda_{i}),$$

and expanding we get:

$$S(\Delta) = \sum (d \ln(d - \lambda_i) - \lambda_i \ln(d - \lambda_i)).$$

**HW18:** Find a formula for the Euler characteristic  $\chi(L_{m,n})$ .

We propose the formula  $\chi(L_{m,n}) = 1 - (m-1)(n-1)$ . We can prove this by using the fact that the Euler characteristic is equal to the number of vertices minus the number of edges:

$$\chi = |V| - |E|.$$

The number of vertices is mn. The number of edges is:

$$n(m-1) + m(n-1) = mn - n + mn - m = 2mn - m - n.$$

Now, we can compute:

$$\chi = |V| - |E| = mn - (2mn - m - n) = -mn + m + n.$$

Observe, we can simplify the proposed formula:

$$\chi = 1 - (m-1)(n-1) = 1 - (mn - m - n + 1) = -mn + m + n.$$

Therefore, both expressions agree, and the formula holds.

**HW19:** Compute the von Neumann entropy of the first graph (see drawing), along with the entropy of the path graph  $P_3$ . Then compare their combined entropy to the entropy of  $P_7$ .



First, we compute the Laplacian for the first graph. The degree matrix is:

$$D_{\Gamma_1} = \text{diag}(1, 3, 2, 2)$$

The adjacency matrix is:

$$A_{\Gamma_1} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

So  $\Delta_{\Gamma_1} = D - A$  is:

$$\Delta_{\Gamma_1} = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$$

The eigenvalues of this matrix are:

$$\lambda_1 = 0$$
,  $\lambda_2 = 1$ ,  $\lambda_3 = 3$ ,  $\lambda_4 = 4$ 

Therefore, the entropy is:

$$S = \sum_{i} \lambda_{i} \ln \lambda_{i} = (1 \ln 1 + 3 \ln 3 + 4 \ln 4) \approx 0 + 3.295 + 5.545 = 8.84$$

Adding this to our previously calculated entropy for  $P_3$ , we get a total entropy:

$$S_{\text{combined}} = 8.84 + 3.295 = 12.13$$

Now, we can compute the entropy for  $P_7$ . The Laplacian is:

$$\Delta_{P_7} = egin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \ -1 & 2 & -1 & 0 & 0 & 0 & 0 \ 0 & -1 & 2 & -1 & 0 & 0 & 0 \ 0 & 0 & -1 & 2 & -1 & 0 & 0 \ 0 & 0 & 0 & -1 & 2 & -1 & 0 \ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

The eigenvalues of this matrix are:

$$\lambda_1 = 0, \quad \lambda_2 = 0.198, \quad \lambda_3 = 0.753, \quad \lambda_4 = 1.555, \quad \lambda_5 = 2.445, \quad \lambda_6 = 3.247, \quad \lambda_7 = 3.802$$

Therefore, the entropy is:

$$S(P_7) = \sum_{i=1}^{7} \lambda_i \ln \lambda_i \approx 11.25$$

We observe that  $S(P_7) < S_{\text{combined}}$ , meaning the single longer path has lower entropy than the disjoint union.

**HW20:** Questions about Graph Theory project:

- 1. How will you calculate distance? Taking an average might not accurately reflect what you want if a single class is an outlier.
- 2. How is similarity defined? Is there some way to see if STEM or humanities students are taking classes in different disciplines? Which groups are more likely to branch out?
- 3. Similar to my first question: pre-med students take a variety of courses but aren't necessarily utilizing the open curriculum. Is there a way to reflect this?
- 3. How are cross-listed courses being dealt with?

**HW21:** Find all simple graphs of order 4 up to isomorphism. (b) Compute  $L(\Gamma)$  (c) Compute  $S(\Delta_{\Gamma})$ 

• 1. Empty graph (4 single vertices, 0 edges)

		- b) infinite
		- c) 0
•	2.	Single edge (one edge connecting two vertices, others alone)
		<ul><li>b) infinite</li><li>c) 1.38</li></ul>
•	3.	Two disjoint edges (two edges, no vertices shared)
		<ul><li>b) infinite</li><li>c) 2.77</li></ul>
•	4.	Path of length $2$ (three vertices connected in a chain, one vertex alone)
		<ul><li>b) infinite</li><li>c) 3.30</li></ul>
•	5.	Star graph $K_4$ (one center vertex connected to the other three)
		- b) 1.5 - c) 5.5
•	6.	$P_4$ (four vertices connected in a chain)
		- b) 1.67 - c) 5.25
•	7.	$C_4$ (four vertices connected in a square)
		- b) 1.33 - c) 8.32
•	8.	Triangle plus an edge
		- b) 1.33 - c) 8.84
•	9.	Complete graph minus one edge (4 vertices, 5 edges)
		- b) 1.17 - c) 12.47
•	10	). Complete graph $K_4$
		- b) 1 - c) 16.64

**HW22:** Find the difference in the Euler characteristic between





$$\chi = |V| - |E|$$

 $\Gamma_1$  has:

- |V| = 12 vertices
- |E| = 17 edges

 $\Gamma_2$  has:

- |V| = 13 vertices
- |E| = 18 edges

$$\Rightarrow \chi_1 = 12 - 17 = -5$$

$$\Rightarrow \chi_2 = 13 - 18 = -5$$

Therefore, the Euler characteristic is the same for both graphs:

$$\chi(\Gamma_1) = \chi(\Gamma_2) = -5$$

This also matches the relation  $\chi = b_0 - b_1$ , since the graphs are connected  $(b_0 = 1)$  and contain 6 independent cycles  $(b_1 = 6)$ :

$$\chi = 1 - 6 = -5$$

**HW23:** What is the  $\Omega$  index?

The small-worldness of a network can be measured using a coefficient called the sigma index  $(\sigma)$ . It is calculated by comparing the clustering coefficient and characteristic path length of a network to those of an equivalent random network with the same average degree. However, the performance of this index suffers in larger networks.

The omega index  $(\omega)$  is thus a better quantifier of small-worldness. It compares the path length of the network to that of a random graph and the clustering coefficient to that of a regular (lattice-like) graph. The value of  $\omega$  ranges from -1 to 1, where:

•  $\omega \approx -1$ : The network is represented by a lattice and is regular

- $\omega \approx 0$ : The network exhibits small-world properties
- $\omega \approx 1$ : The network behaves like a random graph

**HW24:** Calculate the entropy of the torus graph.

The degree matrix is:

$$D_{\Gamma} = \text{diag}(2, 2, 2, 2)$$

The adjacency matrix is:

$$A_{\Gamma} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

So the Laplacian matrix is:

$$\Delta_{\Gamma} = D_{\Gamma} - A_{\Gamma} = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$$

The eigenvalues of this Laplacian matrix are:

$$\lambda_1 = 0, \quad \lambda_2 = 2, \quad \lambda_3 = 2, \quad \lambda_4 = 4$$

Therefore, the entropy is:

$$S = \sum \lambda_i \ln \lambda_i = 2(2 \ln 2) + (4 \ln 4) \approx 8.31$$