Quantum Graph Entropy and the Phase Space Visualization of Schrödinger's Equation

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Outline

1. Introduction to Entropy in Graph Theory
   - Spectral Graph Theory
   - Von Neumann Entropy
   - Relevance and Applications
   - Approximating the Entropy of Large Matrices
2. Graph Quantum Mechanics and the Von Neumann Entropy of Graphs
   - The Discrete Schrödinger Equation
   - Main Results
     - Von Neumann Entropy of Canonical Graphs
     - Analytical Approximation of Von Neumann Entropy
     - Numerical Approximation of Von Neumann Entropy
3. Visualizing the Schrödinger Equation in Phase Space
   - Solving the Schrödinger Equation
   - Phase Space Visualization

Spectral Graph Theory

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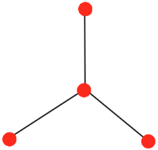
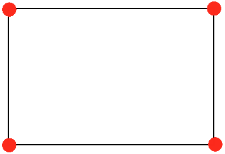
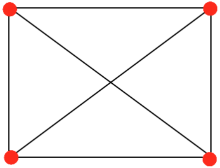






$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Spectral Graph Theory

Definition (The Laplacian Matrix)

Given the **adjacency matrix, A**, and the **degree matrix, D**, for a given graph Γ, the **Laplacian**, $\Delta(\Gamma)$ of the graph is defined as a graph operator that is represented as a symmetric, non-invertible matrix with non-negative diagonal elements and whose rows and columns sum to zero:

$$\Delta = D - A$$

Example (for K_4):

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

Spectral Graph Theory

Theorem (Courant-Fischer)

The eigenvalues and eigenvectors of a symmetric matrix can be thought of in terms of an optimization problem:

$$\lambda_1 = \underset{x \neq 0}{minimum} \frac{x^T L x}{x^T x} \quad v_1 = \underset{x \neq 0}{arg\,minimum} \frac{x^T L x}{x^T x}$$

$$\lambda_2 = \underset{x \perp v_1}{minimum} \frac{x^T L x}{x^T x} \quad v_2 = \underset{x \perp v_1}{arg\,minimum} \frac{x^T L x}{x^T x}$$

$$\ldots$$

Theorem (Bounds on Eigenvalues of the Laplacian)

For a graph Γ with maximal degree d and diameter δ, the growth of the eigenvalues of the Laplacian $\Delta(\Gamma)$ is bounded:

$$\lambda_{k+1} \leq d - 2\sqrt{d-1}\, cos\frac{2\pi k}{\delta}$$

Von Neumann Entropy of Graphs

Definition (The Von Neumann Graph Entropy (VNGE))

Given a Laplacian, Δ, for a graph Γ, the VNGE of Γ is given as

$$S(\Gamma) = -\sum_i \lambda_i \log_2 \lambda_i$$

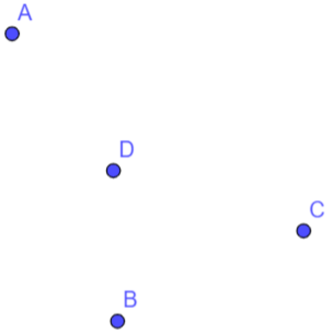
where λ_i are the nonzero eigenvalues of Δ.

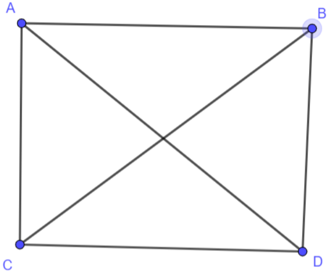
Understanding Von Neumann Entropy

Informally, entropy is a measure of the disorder within a system.

Information entropy (**Shannon**) vs **Quantum entropy** (**Von Neumann**)

Although an exact interpretation of the Von Neumann entropy is still an open question, it is a rough measure of the **complexity** of a graph.





Applications to Machine Learning (Spectral Clustering)

Cluster Analysis is a form of unsupervised machine learning which aims to find natural groupings (i.e. "clusters") within data, such that objects within the same cluster are more similar to each other than to those in different clusters.

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Algorithm:

1. Construct a similarity graph (e.g. kNN) for the data points;
2. Embed the points in a lower-dimensional space using the eigenvectors of the Laplacian;
3. Apply a classical algorithm (e.g. k-means) to the embedding.

Numerical Analysis and Approximations

The **time complexity** of finding the eigenvalues of an $n \times n$ symmetric matrix is $O(n^3)$, so computing the Von Neumann Entropy can be expensive for large matrices.

Proposition (Wihler, Bessire, Stefanov)

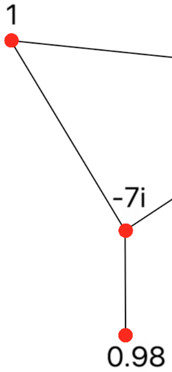
Given a symmetric $m \times m$ matrix A, with $tr(A) \neq 0$, and letting $\omega \in \mathbb{R}^m$ be a vector whose entries are 1 or -1 with equal probability, that is P(1) = P(-1) = 0.5. Then $tr(A) = \mathbb{E}(\omega^T A \omega)$ and we can find an approximation of the trace by taking the mean of N sample computations:

$$tr(A) \approx \frac{1}{N} \sum_{i=1}^{N} \omega_i{}^T A \omega_i$$

Graphs Quantum Mechanics

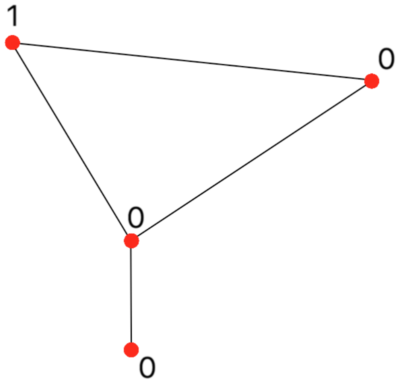
Definition (Quantum State)

Given a graph, Γ, a **Quantum State** is a complex-valued function on the vertex set of the graph, V(Γ).



Definition (Pure Quantum State)

Given a graph, Γ, a **Pure Quantum State** is a **Quantum State** (*a complex valued function on* $V(\Gamma)$) such that only one vertex has a non zero value.



Definition (The Discrete Schrödinger Equation)

Given a graph, Γ, and a quantum state, $|\Psi(t)\rangle$, the **Discrete Schrödinger Equation** is given by

$$\frac{\partial |\Psi(t)\rangle}{\partial t} = i\Delta |\psi(t)\rangle$$

where Δ is the **Graph Laplacian Operator**.

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Now that we have entered the realm of **Quantum Mechanics**, what relevant **questions** can we ask?

Von Neumann Entropy of Graphs

Definition (Recall the Von Neumann Entropy)

Given a Laplacian, Δ, for a graph Γ, the VNGE of Γ is given as

$$S(\Gamma) = -\sum_i \lambda_i \log_2 \lambda_i$$

where λ_i are the eigenvalues of Δ.

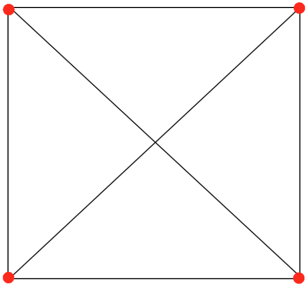
The Von Neumann Entropy of Canonical Graphs

Many canonical graphs have a closed form expression for their entropy in terms of their number of vertices.

Theorem (VNGE of Complete Graphs, A.M.)

Given a Complete Graph, K_n, with n vertices, the entropy of the graph is given as

$$S(K_n) = -n(n-1)\log_2 n$$

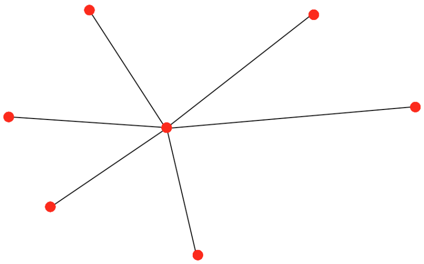


The Von Neumann Entropy of Canonical Graphs

Theorem (VNGE of Star Graphs, D.W.)

Given a Star Graph, S_n, with n vertices, the entropy of the graph is given as

$$S(S_n) = -n \log_2 n$$

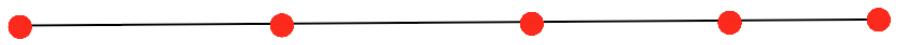


The Von Neumann Entropy of Canonical Graphs

Theorem (VNGE of Path Graphs, A.M., D.W.)

Given a Path graph, P_n, with n vertices, the following asymptotic behavior holds:

$$\lim_{n\to\infty} \frac{S(P_n)}{-2n} = 1$$

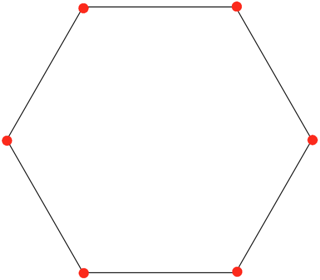


The Von Neumann Entropy of Canonical Graphs

Theorem (VNGE of Cycle Graphs, A.M., D.W.)

Given a Cycle graph, C_n, with n vertices, the following asymptotic behavior holds:

$$\lim_{n\to\infty} \frac{S(C_n)}{-2n} = 1$$



The Polynomial Approximation of Entropy

Definition (Trace Normalized Entropy)

The **Trace Normalized Entropy** of a graph is given as

$$N(\Gamma) = \sum_i \frac{-\lambda_i}{Tr(\Gamma)} \log_2 \frac{\lambda_i}{Tr(\Gamma)}$$

The Polynomial Approximation of Entropy

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Theorem (A.R., D.W.)

The **Trace Normalized Entropy** *of a graph can be approximated using the Taylor series expansion as*

$$N(\Gamma) \approx \sum_{i=0}^{m} c_i Tr(\Delta^{i+1})$$

where m is the order of approximation.

The Numerical Approximation of Entropy using Degree Statistics

Conjecture (Entropy as a Function of $|V|$ and $|E|$, D.W.)

Given a vertex set V and a corresponding edge set, the entropy of a random graph Γ with $|E|$ edges on the given vertex set can be approximated as

$$S(\Gamma) = \sum_{i=1}^{\infty} c_i(|E|^{1/i})$$

where each c_i is a function of $|V|$.

The Numerical Approximation of Entropy using Degree Statistics

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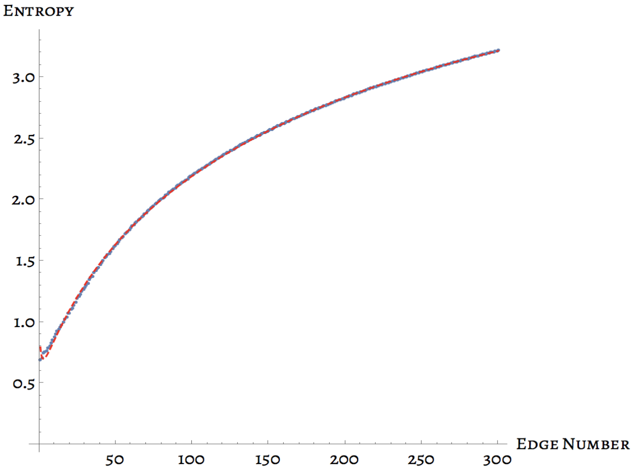
This is very important for understanding the **entropy of glued graphs**.

Evidence

For each vertex set up to $|V| = 29$, we have approximating functions

$$S(\Gamma) \approx c_0 + c_1|E| + c_2|E|^{1/2} + c_3|E|^{1/3} + c_4|E|^{1/4}$$



Future Directions

* Find a generalized approximation of the entropy of a graph in terms of its degree statistics
* Find a general formula for the entropy of gluing
* Establish a Graph Quantum Mechanics analog of the Heisenberg Uncertainty Relations
* Consider the solutions of the Discrete Schrödinger Equation with an added potential

Solving Discrete Schrödinger

Suppose

- Γ is a graph
- $\Psi(t) : V(\Gamma) \longrightarrow \mathbb{C}$ is a time-dependent state
- Δ is the Laplacian matrix of Γ

Observation (Discrete Schrödinger Equation Solved)

Discrete Schrödinger is

$$\frac{\partial |\Psi(t)\rangle}{\partial t} = i\Delta |\Psi(t)\rangle \qquad \longrightarrow$$

And the following is a **solution**:

$$|\Psi(t)\rangle = \exp(i\Delta t) |\Psi(0)\rangle$$

Since $|\Psi(t)\rangle$ is proportional to its derivative.

Phase Space

- **Phase space** is an imaginary "space" representing the system.
- The state of the system is represented as a single point.
- For a graph with n vertices at time t, $|\Psi\rangle$ is a n-dimensional complex vector.
- Therefore the state is a unique point in $2n$-dimensional real space.
- Schrödinger equation describes the **movement** of that point.

> What will the **trajectory** in phase space representing the time evolution look like? Which are **periodic**?

Observation

Eigenstates evolve in orthogonal circles with period

$$T = \frac{2\pi}{\lambda}$$

And radius equal to the coefficient of the eigenstate.

Sketch Proof

This is actually quite obvious—apply basic theorem of matrix exponents to the diagonalization $\Delta = VDV^{-1}$.

$$
\begin{aligned}
|\Psi(t)\rangle &= \exp(i\Delta t)\,|\Psi(0)\rangle \\
&= \begin{bmatrix} | & & | \\ E_1 & \dots & E_n \\ | & & | \end{bmatrix}
\begin{bmatrix} e^{i\lambda_1 t} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & e^{i\lambda_n t} \end{bmatrix}
\begin{bmatrix} | & & | \\ E_1 & \dots & E_n \\ | & & | \end{bmatrix}^{-1}
\begin{bmatrix} | \\ \Psi(0) \\ | \end{bmatrix}
\end{aligned}
$$

Each exponent on the diagonal "rotates" separately and corresponds to a single eigenstate.

Toroidal Manifold Interpretation

- Each eigenstate describes independent $\mathbb{S}^1$.
- Trajectory therefore lives on $\mathbb{S}^1 \times \cdots \times \mathbb{S}^1 = \mathbb{T}^n$, the *n-torus*, embedded in $2n$-dimensional phase space.
- Call this embedding $\mathcal{M}$.

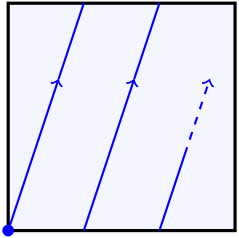
Theorem (A.M)

For $|\Psi(0)\rangle = c_1 E_1 + \cdots + c_n E_n$ initial state. If eigenvalues of eigenstates with nonzero coefficients are all commensurable, $|\Psi\rangle$ is periodic. Otherwise, $|\Psi\rangle$ is non-periodic and the closure of the trajectory of $|\Psi\rangle$ is equal to $\mathcal{M}$.

*Note: p and q **commensurable** when $p/q \in \mathbb{Q}$.*

Sketch Proof (Part 1)

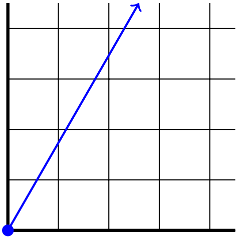
Represent each $\mathbb{S}^1$ as a line segment with ends identified. $\mathcal{M}$ becomes a solid n-cube, and the trajectory a straight line wrapping inside it.



Its speed along each axis is determined by its period along that $\mathbb{S}^1$.

Sketch Proof (Part 2)

Now "unwind" each $\mathbb{S}^1$ into an $\mathbb{R}$, and the n-cube into $\mathbb{R}^n$. The trajectory is a straight line ray through the point $(\lambda_1, \dots, \lambda_n)$.



Theorem (Known Result)

Ray through $(p_1, \dots, p_n)$ under quotient map $q : \mathbb{R}^n \longrightarrow \mathbb{R}^n/\mathbb{Z}^n$ dense if and only if nonzero p's all incommensurable.

All states on graphs with integer eigenvalues are periodic!

THANK YOU!

References

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[3] Wihler, Thomas P, et al. "Computing the Entropy of a Large Matrix." Journal of Physics A: Mathematical and Theoretical, vol. 47, no. 24, 2014, p. 245201., doi:10.1088/1751-8113/47/24/245201.