Developments on Graph Quantum Mechanics, Graph de Rham Calculus, and Discrete Morse Theory

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Introduction

The general goal of this project is to develop discrete analogues of results in mathematical physics. In particular, we connect notions from physics such as entropy and quantum states to the realm of graph theory, a mathematical abstraction commonly used to model networks in computer science, engineering, and some other fields. Our graph theoretical model of quantum mechanics interacts with different areas such as network theory, linear algebra, and the topology of graphs.

Preliminaries

An *graph* Γ is a pair (V, E) where V is a set of *vertices* and $E \subseteq V \times V$ is a set of *edges* connecting vertices to one another. A graph is *oriented* if we assign directions to each edge.

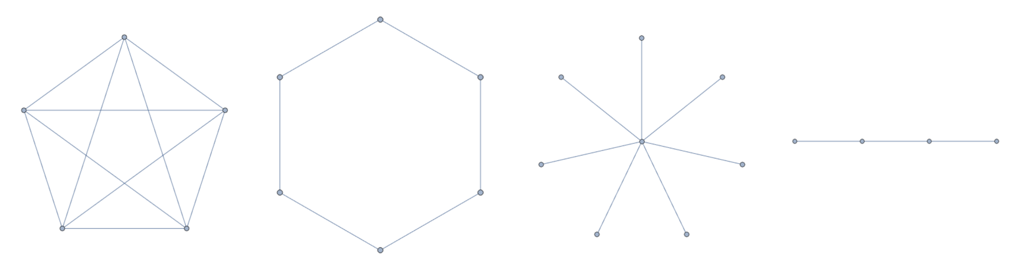

Figure 1: Some standard graphs with particular numbers of vertices. From left to right: the complete graph K_5, the cycle graph C_6, the star graph S_8, and the path graph P_4.

Definition (Incidence Matrix)
Let Γ be an oriented graph. The incidence matrix I of Γ is a $|V| \times |E|$-matrix defined by

$$I(k,l) = \begin{cases} -1 & \text{if } e_l \text{ starts at } v_k \\ 1 & \text{if } e_l \text{ ends at } v_k \\ 0 & \text{otherwise.} \end{cases}$$

Graph Laplacian

We can associate with each graph a matrix called the *graph Laplacian*, an analogue of the Laplacian from calculus, which is invariant under change of orientation and thus well-defined for undirected graphs. We can then study how the Laplacian changes under what is called *interface gluing*.

Definition (Graph Laplacian)
For a graph Γ with incidence matrix I, the *Laplacian* Δ of the graph is the $|V| \times |V|$-matrix defined by

$$\Delta = II^t$$

where t denotes the transpose of a matrix.

Definition (Interface Gluing)
Let Γ_1 and Γ_2 be two graphs. If Γ_1^∂ and Γ_2^∂ are two isomorphic subgraphs of Γ_1 and Γ_2 respectively, then $\partial\Gamma \cong \Gamma_1^\partial \cong \Gamma_2^\partial$ is an *interface* of the graphs Γ_1 and Γ_2. The *interface gluing* of the two graphs is the graph $\Gamma_1 \sqcup_{\partial\Gamma} \Gamma_2$ resulting by gluing along the interface.

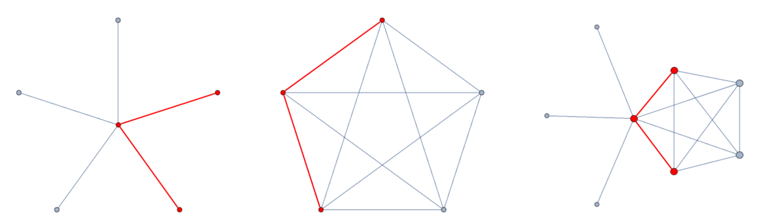

Figure 2: The gluing of S_5 and K_5 along the interface of $\partial\Gamma = P_3$.

Definition (k-subdirect sums)
Let A and B be two square matrices of order n_1 and n_2, respectively, and let k be an integer such that $1 \leq k \leq \min(n_1, n_2)$. Let A and B be partitioned into 2×2 blocks as follows:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

where A_{22} and B_{11} are square matrices of order k. The following square matrix has order $n = n_1 + n_2 - k$, and is called the *k-subdirect sum* of A and B and denoted by $C = A \oplus_k B$.

$$C = \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} + B_{11} & B_{12} \\ 0 & B_{21} & B_{22} \end{bmatrix}.$$

Theorem
Let Γ_1, Γ_2 be two graphs. Then the following holds

$$\Delta_{\Gamma_1 \sqcup_{\partial\Gamma} \Gamma_2} = \Delta_{\Gamma_1} \oplus_n \Delta_{\Gamma_2}$$

if and only if the interface is a disjoint union of vertices.

Von Neumann Graph Entropy

In classical information theory, Shannon entropy quantifies the uncertainty in a classical random variable. Von Neumann entropy can be thought of as the quantum counterpart of Shannon entropy, as it deals with probability distributions over quantum states. Von Neumann graph entropy is the discrete analogue of this concept, and it is interpreted as a rough measure of the complexity of a graph.

Definition (Entropy)
Let Γ be a graph and the nonzero eigenvalues of the Laplacian be given by λ_i, for $1 \leq i \leq n = |V|$. Then the *Von Neumann graph entropy* (VNGE) of Γ is given by

$$S(\Gamma) = -\sum_{i=1}^{n} \lambda_i \log_2 \lambda_i$$

and the *trace normalized entropy* of a graph Γ is given as

$$N(\Gamma) = \sum_{i=1}^{n} \left(\frac{-\lambda_i}{\mathrm{Tr}(\Gamma)} \log_2 \left(\frac{\lambda_i}{\mathrm{Tr}(\Gamma)} \right) \right).$$

Theorem (Entropy of Standard Graphs)
For complete and star graphs, the VNGE is provided by

$$S(K_n) = -n(n-1)\log_2 n \quad \text{and} \quad S(S_n) = -n \log_2 n.$$

For path and cycle graphs, the VNGE exhibits the limiting behavior

$$\lim_{n\to\infty} \frac{S(P_n)}{-2n} = 1 \quad \text{and} \quad \lim_{n\to\infty} \frac{S(C_n)}{-2n} = 1.$$

Theorem (Trace Normalized Entropy Approximation)
The *trace normalized entropy* of a graph Γ can be approximated using the Taylor series expansion given by

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

where m is the order of approximation and c_i is a coefficient dependent on m and $|V|$.

Phase Space of the Schrödinger Equation

We define an analogue of the quantum mechanical Schrödinger equation on a graph with n vertices. The solution of this equation is a vector evolving in time with n complex entries (or $2n$ real entries), in what is known as *phase space*. Here, we study the trajectory taken by the solution.

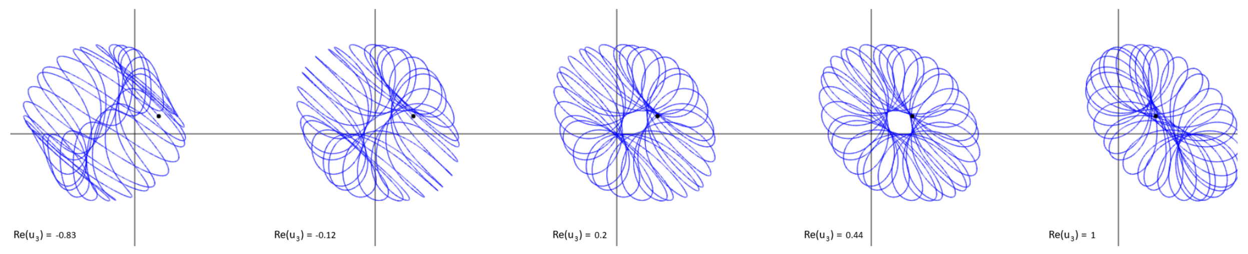

Figure 3: The solution of the Schrödinger equation projected onto a plane determined by vectors $\vec{u}, \vec{v} \in \mathbb{C}^{|V|}$. In the figure, we are increasing the real-part of the component u_3 of $\vec{u}$.

Definition (Quantum State)
A *quantum vertex state* (resp. *quantum edge state*) assigns a complex value to each vertex (or edge) on a graph. It is a vector in $\mathbb{C}^{|V|}$ or $\mathbb{R}^{2|V|}$ (or $\mathbb{C}^{|E|}$ or $\mathbb{R}^{2|E|}$).

Definition (Discrete Schrödinger Equation)
Let $|\Psi(t)\rangle$ be a quantum vertex state that evolves in time t with initial condition $|\Psi(0)\rangle$. Then the *discrete Schrödinger equation* and its solution is given by

$$\frac{\partial\,|\Psi(t)\rangle}{\partial t} = i\hbar\Delta\,|\Psi(t)\rangle \quad \longrightarrow \quad |\Psi(t)\rangle = \exp(i\hbar\Delta t)\,|\Psi(0)\rangle\,.$$

Theorem
Let $\{E_i\}_{i=1}^n$ be the eigenstates of Δ, and $|\Psi(0)\rangle = c_1E_1 + \cdots + c_nE_n$ the initial state. If the eigenvalues of eigenstates with non-zero coefficients are all commensurable, $|\Psi\rangle$ is periodic. Otherwise, $|\Psi\rangle$ is non-periodic and the closure of the trajectory of $|\Psi\rangle$ is a m-dimensional torus embedded in $\mathbb{R}^{2|V|}$, where $m = |V| - k$, where k is the number of commensurable eigenvalues.

Discrete Morse Theory

Smooth Morse theory is the study of smooth functions with non-degenerate critical points on smooth manifolds. Within the subject, the critical points allow us to understand important properties of the manifold the function is defined on. Robin Forman in 2002 adapted an analogue for CW complexes, and here we focus on developing the subject for graphs.

A *discrete Morse function* on $\Gamma = (V, E)$ is an assignment $V \cup E \to \mathbb{R}$ such that at every vertex, at most one connected edge as lower value (if there are none, the vertex is *critical*), and at every edge, at most one endpoint has higher value (if there are none, then the edge is *critical*).

A discrete Morse function f on a graph Γ gives rise a directed graph called the *gradient flow* Γ_f, an oriented graph where $e = (v, w) \in E_{\Gamma_f}$ only if $f(v) < f(e)$.

Figure 4: (Left) A discrete Morse function on a graph. (Right) The resulting gradient flow from the assignment.

Theorem
Let Γ_o be a directed graph and Γ be its underlying undirected graph. Then $\Gamma_o = \Gamma_f$ for some discrete Morse function f on Γ if and only if

1. no two edges share a tail, and
2. there are no directed loops.

Theorem
Let f be a discrete Morse function on a graph Γ. Then

1. An edge is a critical cell of f on Γ if and only if it is undirected in Γ_f.
2. A vertex is a critical cell of f on Γ if and only if it is a sink in Γ_f.

If we denote by $\mathsf{Morse}(\Gamma)$ be the set of all discrete Morse functions that can be defined on a graph Γ, then a natural sense of equivalence on the set is

$$f \sim_\Gamma g \iff \Gamma_f \cong \Gamma_g.$$

Theorem (Weak Morse Inequalities)
Let f be a discrete Morse function on a graph Γ. Let $c_0(f)$ denote the number of critical vertices, and $c_1(f)$ the number of critical edges. Then

- $b_i(\Gamma) \leq c_i(f)$ for $i \in \{0, 1\}$
- $\chi(\Gamma) = c_0(f) - c_1(f)$

Graph de Rham Calculus

When one applies I^t to a vertex state, one gets an edge state. The way that I^t acts is quite simple: it assigns to each edge the difference of values on that edge's vertices. Thus, I^t acts as an analogue of gradient differential operator. Here, we develop a corresponding theory of integration.

Definition (Vertex Integral)
Let f be a vertex state on Γ. The **vertex integral of f over Γ** is given by

$$\int_{\partial\Gamma}^{\bullet} f = \sum_{v_i \in V} f(v_i) d_n(v_i),$$

where $d_n(v_i)$ is the *net degree*, i.e. incoming minus outgoing edges.

Definition (Edge Integral)
Let F be an edge state on Γ. The **edge integral of F over Γ** is given by

$$\int_{\Gamma}^{-} F = \sum_{e_i \in E} F(e_i).$$

Theorem (Stokes' Theorem for Graphs)
Let f be a vertex state on an oriented graph Γ. Then

$$\int_{\partial\Gamma}^{\bullet} f = \int_{\Gamma}^{-} I^t f.$$

Future Directions

- **Conjecture:** If Γ is a random graph with a fixed number of vertices, then $N(\Gamma)$ upon prescribing k-many edges may be approximated as $\sum_{i=1}^{\infty} c_i\sqrt{k}$, where each c_i is a function dependent on $|V|$.
- **Conjecture:** The number of equivalence classes of discrete Morse functions for a graph Γ such that there are b_1-many critical edges is dependent on the number of unique (non-isomorphic) spanning trees.
- What properties of graph integration are invariant under orientation?

Acknowledgements

We would like to thank Andy Anderson for helping us to access the AC computing cluster, Prof. Alejandro Morales and the UMass REU discrete geometry groups for their valuable feedback, and Prof. Ivan Contreras for his mentorship at every step of the way. We also thank the Gregory Call and SURF programs for funding this project.

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