Spectral and Stochastic Solutions to Boundary Value Problems on Magnetic Graphs

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Abstract.
A magnetic graph is a graph G equipped with a signature structure σ on its edges. Magnetic graphs have been an important tool in the study of quantum mechanics since at least 1993, with the publication of a classic paper by Lieb and Loss. Among many other things, these graphs help us model simple electromagnetic systems. In this talk, we will explore the discrete magnetic Laplace operator $\mathcal{L}_G^\sigma$, a difference operator for complex-valued functions on the vertices of G. We will pose some discrete boundary value problems associated to this operator, and adapt two classic techniques to the setting of magnetic graphs to solve them. The first technique uses the spectral properties of the operator, and the second technique utilizes random walks adapted to this particular setting. Throughout, we will prove some useful results including a Green's identity, mean value characterization of harmonic functions, and extensions of the solution techniques to Kronecker product graphs.

What is a magnetic graph?

- $G = (V(G), E(G))$ undirected, finite, no loops or multiple edges
- The **oriented edges** of G

  $$E^{\mathrm{or}}(G) := \{(u,v),(v,u) : \{u,v\} \in E(G)\}.$$

- A **signature** on G is a map

  $$\sigma : E^{\mathrm{or}}(G) \to S^1 : (u,v) \mapsto \sigma_{uv}$$

  s.t. $\sigma_{vu} = \overline{\sigma_{uv}}$.
- Gives notion of **direction** for the edges of G
- A **magnetic graph** is a pair (G, σ).

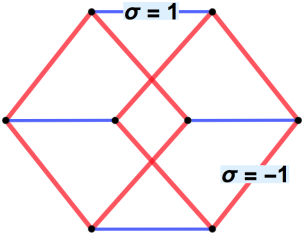

Figure: Example graph with example signature taking real values, illustrated by edge coloring

What is a Discrete Laplace Operator?

- A general **weight function** on G is some function w_{uv} on $V(G) \times V(G)$, usually with some restrictions like positivity or symmetricity.
- A **discrete Laplace operator** associated to w is a linear operator L on the function space $\ell_2(V(G)) := \{f : V(G) \to \mathbb{C}\}$ of the form

$$(Lf)(u) = \sum_{v \in V(G)} w_{uv}(f(u) - f(v)) \tag{1}$$

- w is chosen so that L inherits properties of classical Laplace operator Δ for differentiable functions
- **Wardetsky** has studied the properties which a general discrete laplacian may inherit from the classical case, **"no free lunch"**
- The **combinatorial Laplacian** chooses $w_{uv} = 1 \iff u \sim v$, 0 otherwise. We build off of this.

Combinatorial Laplace operator (Example)

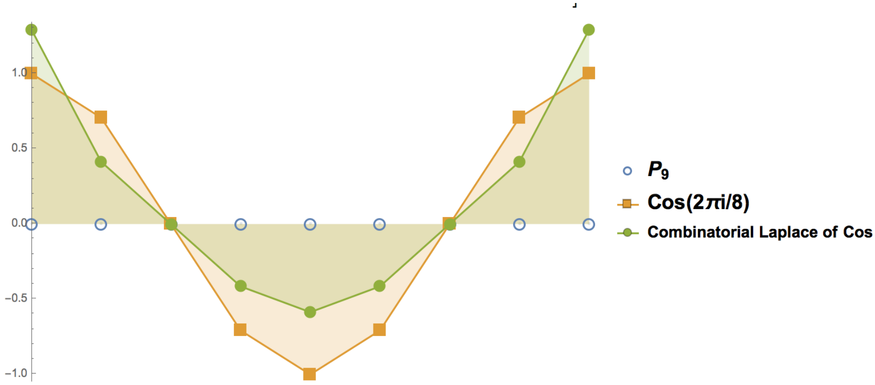

Figure: A Cosine function on a 9 vertex path alongside its combinatorial Laplacian in green

The magnetic Laplace operator

- The **magnetic Laplace operator** extends (1) to a magnetic graph (G, σ).
- Let $f \in \ell_2(V(G))$. Define $\mathcal{L}_G$ by

$$(\mathcal{L}_G f)(u) = \sum_{v \sim u} f(u) - \sigma_{uv} f(v). \quad (2)$$

  This operator is identified with a **Hermitian** matrix $\mathcal{L}_G$. It is a **self-adjoint** operator.
- If $H \subsetneq V(G)$ is a subset of vertices, L_H is its **magnetic Dirichlet Laplacian** and $\frac{\partial}{\partial \eta}$ is its **normal derivative** operator. These measure 'flow' of a function on G into and out of H, resp.
- ∂H is the **vertex boundary** of H, $\overline{H} := H \cup \partial H$.

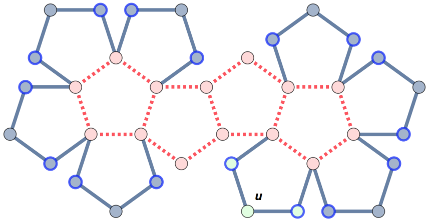

Figure: A Dodecahedron graph with subset H in red, vertex boundary in bright blue

Results (1), Identities

Theorem (Magnetic Mean Value Property)

A function $f \in \ell_2(V(G))$ is harmonic on a magnetic graph (G, σ) if and only if at each vertex $u \in V(G)$, the following holds:

$$f(u) = \frac{1}{d_u^G} \Bigg(\sum_{\substack{v \sim u \\ v \in G}} \sigma_{uv} f(v) \Bigg).$$

Theorem (Magnetic Green's Identity)

Let (G, σ), H be as before and $f, g \in \ell_2(V(\overline{H}))$. Then the following holds:

$$\sum_{u \in H} (\mathcal{L}_{\overline{H}} f)(u)\overline{g(u)} - f(u)\overline{(\mathcal{L}_{\overline{H}} g)(u)} = \sum_{u \in \partial H} f(u)\overline{\frac{\partial g}{\partial \eta}(u)} - \frac{\partial f}{\partial \eta}(u)\overline{g(u)}.$$

Results (2), Green's Functions

Lemma

Let (G, σ) be a connected magnetic graph, and suppose $H \subsetneq V(G)$ is a proper subset of vertices which induces a connected subgraph in G. Then L_H is an invertible matrix.

Theorem (Green's Function Formula)

Let G be a finite connected graph without loops or multiple edges, and let $H \subsetneq V(G)$ be a proper subset of k vertices which is assumed to induce a connected subgraph. Let $\{e_i\}_{i=1}^m$ be an orthonormal basis of $\ell_2(H)$ of eigenvectors of L_H associated to eigenvalues $\{\lambda_i\}_{i=1}^m$ counted with multiplicity. Let L_H^{-1} be interpreted as a function on $H \times H$. We have the following

$$L_H^{-1}(i,j) = \sum_{k=1}^{m} \frac{1}{\lambda_k} e_k(i)\overline{e_k(j)}$$

where $(i,j) \in H \times H$ (we use slightly different notation for vertices in H here to be consistent with the $\{e_i\}$ notation).

Results (3), Poisson Problem

Magnetic Poisson Problem Let $f \in \ell_2(H)$ and $g \in \ell_2(\partial H)$ be given functions. We wish to find a function $\Psi \in \ell_2(\overline{H})$ for which

$$\begin{cases} (\mathcal{L}_G \Psi)(u) = f(u) & u \in H \\ \Psi(u) = g(u) & u \in \partial H \end{cases} \tag{3}$$

We shall solve this problem using a **spectral theoretic solution**, whose combinatorial origins are due to **Chung**.

Theorem (Spectral Theoretic Solution)

Let $\{e_i\}_{1 \le i \le k}$ be an orthonormal basis of $\ell_2(H)$ of eigenvectors for L_H, associated to real eigenvalues $\{\lambda_i\}_{1 \le i \le k}$, counted with multiplicity. Extend this system on H to a family $\{\widetilde{e}_i\}$ on $\overline{H}$ by setting $\widetilde{e}_i \equiv 0$ on ∂H. The unique solution to (3) may be explicitly given by

$$\Psi(w) = \begin{cases} (L_H^{-1} f)(w) - \sum_{i=1}^{m} \frac{e_i(w)}{\lambda_i} \left[\sum_{u \in \partial H} \overline{\frac{\partial \widetilde{e}_i}{\partial \eta}(u)} g(u) \right] & w \in H \\ g(w) & w \in \partial H \end{cases}.$$

Results (4), Stochastic Solution 1

The **magnetic Dirichlet problem** is stated as follows: Let (G, σ) be a **simple** and **connected** magnetic graph and let H be a proper subset in $V(G)$ which induces a connected subgraph. Let $f \in \ell_2(\partial H)$ be a given boundary condition. We wish to find a function $\Psi \in \ell_2(\overline{H})$ for which

$$\begin{cases} (\mathcal{L}_G \Psi)(u) = 0 & u \in H \\ \Psi(u) = f(u) & u \in \partial H \end{cases} . \tag{4}$$

Theorem (Dirichlet Solution 1)

Let G, H, f, Ψ be as in (4). Let S_t be a random walk with associated initial distribution μ_0. The unique solution to (4) may be given by

$$\Psi(u) = \mathbb{E}[f(\widetilde{S_T}) \prod_{i=1}^{T} \sigma_{S_{i-1}S_i} : \mu_0 = \delta_u], \quad u \in \overline{H} \tag{5}$$

where $\widetilde{S}_t$ is the modified random walk which stops once reaching the boundary at step T.

Magnetic Lifts

Let (G, σ) be a magnetic graph. Further assume that σ takes values strictly in $\mathbf{S}^1_p$ for some integer $p \geq 2$. Write $\mathbf{S}^1_p = \{\omega_i\}_{i=0}^{p-1}$ We define the **lift** of G to be the non-magnetic graph $\widehat{G}$ consisting of vertex set $G \times \mathbf{S}^1_p$ and edges defined by

$$(u, \omega_i) \sim (v, \omega_j) \text{ in } \widehat{G} \iff u \sim v \text{ in } G \text{ and } \omega_j = \omega_i \sigma_{uv}.$$

The subsets $G \times \{\omega_i\} \subsetneq V(\widehat{G})$ for each fixed $\omega_i \in \mathbf{S}^1_p$ are called the **levels** of the **magnetic lift**.
Current **research questions** concern deducing properties of $\widehat{G}$ determined by properties of G and σ.

Magnetic Lifts (Illustration)

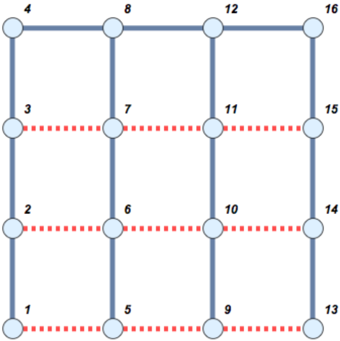

Figure: A grid graph, with signature 1 on the blue edges and signature -1 on the dotted red edges.

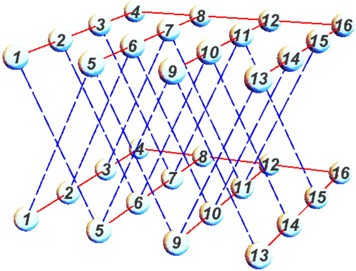

Figure: The magnetic lift associated to the graph on the left; visualized in three dimensions to emphasize the 'level' structures

Results (5), Stochastic Solution 2

Theorem

Let G, H, f, Ψ be as in (4). Assume further that σ takes values in some $\mathbf{S}_p^1 = \{\omega_i\}_{i=0}^{p-1}$ for $p \geq 2$ and that the lift $\widehat{G}$ is connected and not bipartite. Let S_t be a random walk on $\widehat{G}$ on vertices of the form $S_t = (u_t, \sigma_t)$, with associated initial distribution μ_0 on the lift $\widehat{G}$. The unique solution to (4) may be given by

$$\Psi(u) = \mathbb{E}[f(\widetilde{u_T})\sigma_T : \mu_0 = \delta_{(u,\omega_0)}], \quad u \in \overline{H} \tag{6}$$

where $\widetilde{S}_t$ is the modified random walk process formulated in the previous slide.

Open Questions & Acknowledgements

- Which solution technique can be considered more 'efficient' in the computational sense?
- In what way(s) do magnetic lifts simplify the problem, if at all?
- How can we teach these techniques to a computer and implement them on a larger scale?

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