Boundary Value Problems and Green's Functions on Magnetic Graphs

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What is a magnetic graph?

Let $G = (V, E)$ be a finite simple graph, with vertex set V and an edge set G. The set of *oriented edges* is given by

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

A *signature* on G is a map

$$\sigma : E^{or}(G) \to \{z \in \mathbb{C} : |z| = 1\} : (u, v) \mapsto \sigma_{uv}$$

satisfying $\sigma_{uv} = \sigma_{vu}^{-1} = \overline{\sigma_{vu}}$. A *signed* or *magnetic graph* is a graph G equipped a signature structure.

Discrete Laplacians

Graphs serve as extremely useful discrete analogues of continuous domains, often serving as good settings for numerical approximations to solutions of partial differential equations. We investigate the discrete cousin of the classical Laplacian operator, in both unsigned and signed cases. Let $G = (V, E)$ be a finite simple graph, and fix an enumeration of the vertex set $V = \{v_i\}_{i=1}^n$. The *combinatorial* or *discrete Laplacian* of the graph G is the $n \times n$ matrix defined by

$$\mathcal{L}G(i,j) = \begin{cases} d_{v_i} & i = j \\ -1 & v_i \sim v_j \\ 0 & \text{otherwise} \end{cases}$$

where (i) d_{v_i} means the degree of or number of vertices adjacent to the vertex v_i, and (ii) $v_i \sim v_j$ means the two vertices are adjacent. If we have $f : V \to \mathbb{C}$, we may write it as a column vector with respect to the fixed enumeration. The Laplacian of f is then given by the matrix product

$$\mathcal{L}f = (\mathcal{L}G)f.$$

We introduce a boundary value problem on a graph. Suppose we have a graph G, and a proper subgraph H. We define L_H to be the principal submatrix of $\mathcal{L}G$ indexed by the rows and columns of H, with respect to the fixed enumeration. Let

$$V^*(H) := \{x \in V(G) : \{x, y\} \in E(G)\ y \in V(H), x \notin H\}$$

and let $\overline{H}$ be the subgraph in G induced by $V(H) \cup V^*(H)$. Let $f : V^*(H) \to \mathbb{C}$, $g : V(H) \to \mathbb{C}$ be given. The Poisson problem is to find $u : V(H) \cup V^*(H) \to \mathbb{C}$ satisfying

$$\begin{cases} \mathcal{L}u(v) = g(v) & v \in V(H) \\ u(v) = f(v) & v \in V^*(H) \end{cases}$$

The case when $g \equiv 0$ is called the Dirichlet Problem.

The Magnetic Setting

Suppose we have a graph G with a proper subgraph H, defined as above with enumerated vertex set, with a signature σ. We work in the space of functions

$$\ell_2(V(G)) := \{f : V(G) \to \mathbb{C}\}$$

which is naturally isomorphic to $\mathbb{C}^{(\#\text{ vertices in } G)}$, and inherits the natural inner product structure. Define the *magnetic Laplacian* of G to be the $n \times n$ matrix given by

$$\mathcal{L}_\sigma^G(i,j) = \begin{cases} d_{v_i} & i = j \\ -\sigma_{v_i v_j} & v_i \sim v_j \\ 0 & \text{otherwise} \end{cases}$$

noting that this matrix is Hermitian. We define L_σ^H to be the principal submatrix of $\mathcal{L}_\sigma^G$ indexed by the rows and columns of H, with respect to the fixed enumeration. Define the *normal derivative* to be the operator $\frac{\partial}{\partial\eta}$ on $\ell_2(V(\overline{H}))$ given by

$$\frac{\partial f}{\partial \eta}(x) = \sum_{\substack{y \sim x \\ y \in V(H)}} f(x) - \sigma_{xy} f(y).$$

Abstract

Let G be a finite simple graph. We impose on G the additional structure of a signature, a function which maps edges into the set of complex numbers of modulus 1. This induces a second-order difference operator for complex-valued functions defined on the vertex set of G which is a discrete analogue of the classical Laplacian, and consequently discrete boundary value problems on proper and sufficiently connected subgraphs of G. We construct a solution to Poisson type problems and explore some applications, including the role of discrete Green's functions in constructions of solutions. These structures and problems arise in many physical models where discrete domains (namely, graphs) can more efficiently describe continuous regions; in particular, those of quantum mechanics, where a signature structure helps to describe atomic structures with the presence of magnetic potential.

Illustrating the Discrete Dirichlet Problem using *Mathematica*

We illustrate solutions to the combinatorial and magnetic Dirichlet problems subjected to the same boundary condition. Our domain of interest is an 8×8 lattice, denoted G, and we study the Dirichlet problem on the subgraph defined to be the 6×6 interior of the lattice, denoted H (see *Discrete Laplacians*). We shall pose both combinatorial and magnetic problems on this domain; in the case of the magnetic problem, we define a signature σ on H by setting $\sigma = 1$ on horizontal edges and $\sigma = -1$ on vertical edges. Let us define a boundary condition in the form of a sinusoidal curve f, created by wrapping one period of the sine function around the boundary.

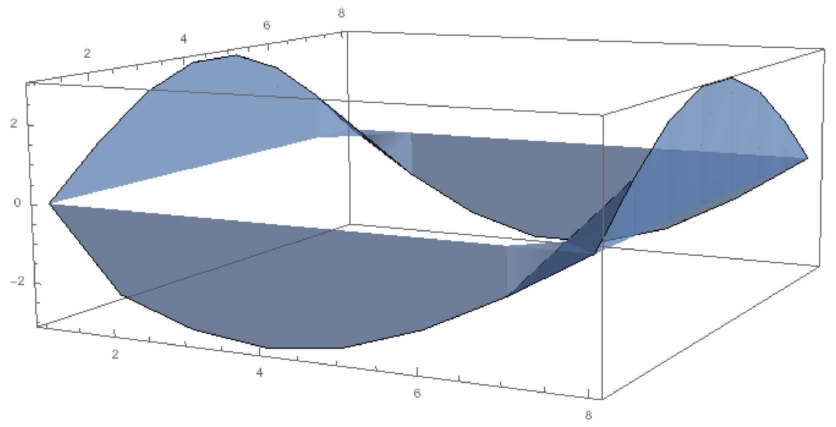


Figure: The boundary function f, with discrete plot points joined to form a curve.

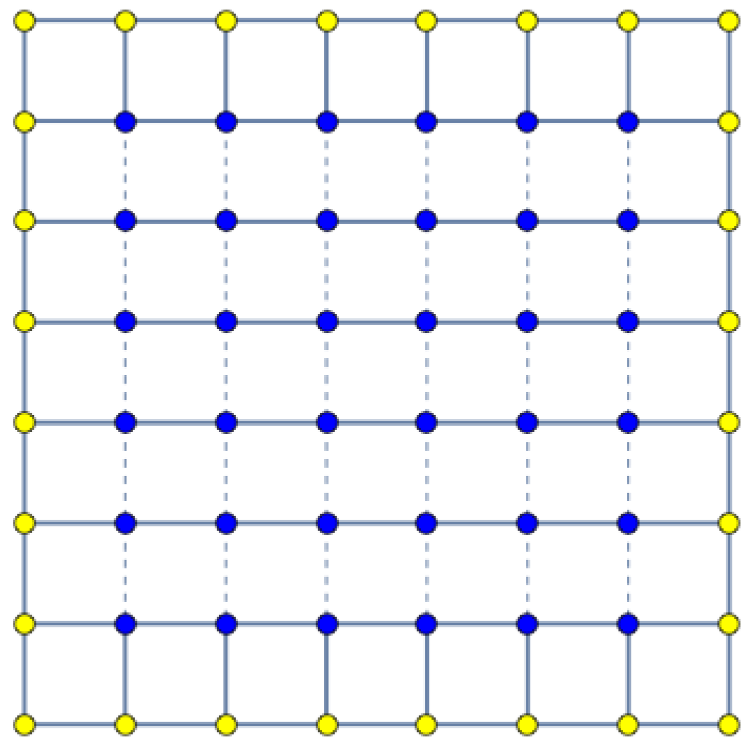
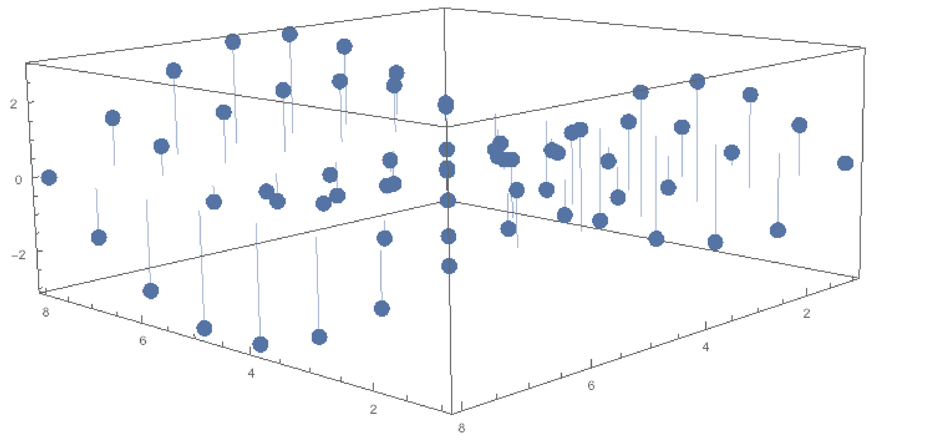


Figure: The graph G, with $V^*(H)$ in yellow, and negatively signed edges dashed.

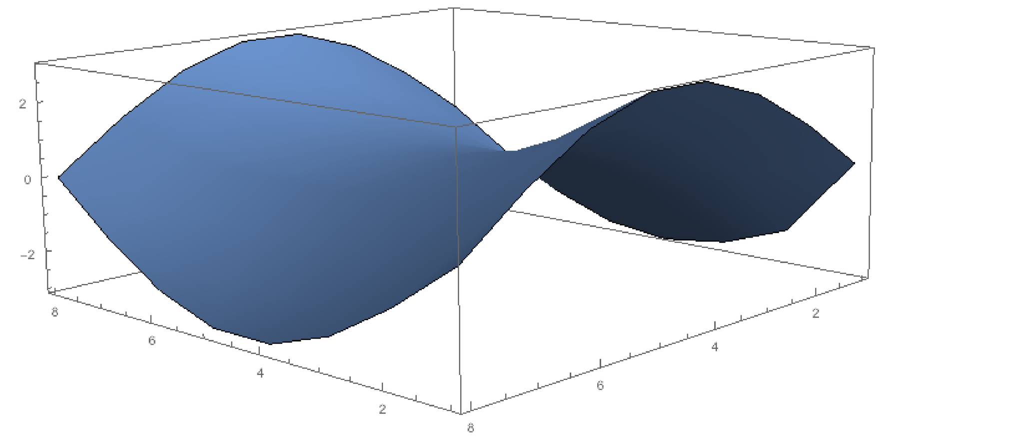
We wish to identify solutions u, v, defined on G to the following problems:

$$\begin{cases} (\mathcal{L}u)(x) = 0 & x \in V(H) \\ u(x) = f(x) & x \in V^*(H) \end{cases} \qquad (1) \qquad\qquad \begin{cases} (\mathcal{L}_\sigma^G v)(x) = 0 & x \in V(H) \\ v(x) = f(x) & x \in V^*(H) \end{cases} \qquad (2)$$

Problem (1) is the combinatorial problem which neglects signature, and problem (2) is the magnetic problem. First, we consider (1). To find the function u, we use techniques seen in *Discrete Green's Functions* by Chung similar to the magnetic solution to (4). Using the DiscretePlot3D tool in *Mathematica*, we have

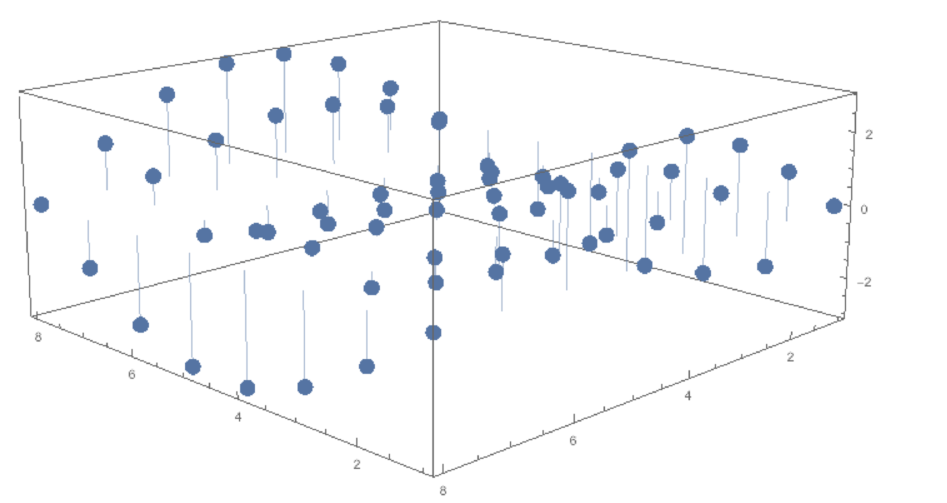


(a) The solution u defined on the whole lattice, plotted discretely

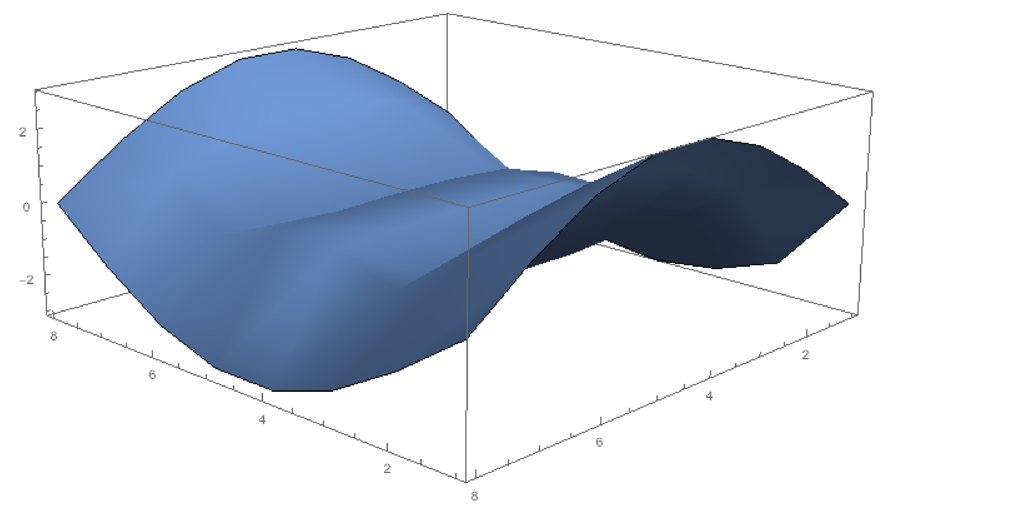


(b) The solution u, defined on the whole lattice, with plot points joined as a surface

Next we consider the magnetic problem (2). Using the techniques described in the results, we are able to produce the solution v, illustrated below using DiscretePlot3D in *Mathematica*:



(a) The solution v defined on the whole lattice, plotted discretely



(b) The solution v, defined on the whole lattice, with plot points joined as a surface

Result 1: Solution to the Magnetic Poisson Problem

Suppose G is a finite, simple signed graph, and H is a proper, connected subgraph of G. Given $g \in \ell_2(V(\overline{H}))$, $f \in \ell_2(V^*(H))$, we wish to find a function $u \in \ell_2(V(\overline{H}))$ so that

$$\begin{cases} (\mathcal{L}_\sigma^{\overline{H}} u)(v) = g(v) & v \in V(H) \\ u(v) = f(v) & v \in V^*(H) \end{cases}$$

We obtain u by finding $u_1, u_2 \in \ell_2(V(\overline{H}))$ which solve

$$\begin{cases} (\mathcal{L}_\sigma^{\overline{H}} u_1)(v) = 0 & v \in V(H) \\ u_1(v) = f(v) & v \in V^*(H) \end{cases} \quad (3) \qquad \begin{cases} (\mathcal{L}_\sigma^{\overline{H}} u_2)(v) = g(v) & v \in V(H) \\ u_2(v) = 0 & v \in V^*(H) \end{cases} \quad (4)$$

so that $u = u_1 + u_2$. Under our assumptions on the domains, unique solutions will exist. We have two theorems giving constructions of the solutions.

Theorem

Let $\{\phi_i\}_{1 \le i \le m}$ be an orthonormal basis of $\ell_2(V(H))$ of eigenvectors of L_σ^H, with associated eigenvalues $\{\lambda_i\}_{1 \le i \le m}$. We extend each ϕ_i to $\tilde{\phi}_i$ agreeing with ϕ_i on $V(H)$ and $\tilde{\phi}_i \equiv 0$ on $V^*(H)$ for $1 \le i \le m$. The solution to (3) is given by

$$u_1(z) = \begin{cases} \sum_{i=1}^m \frac{\phi_i(z)}{\lambda_i} \left[\sum_{x \in V^*(H)} \overline{\frac{\partial \tilde{\phi}_i}{\partial \eta}(x)} f(x) \right] & z \in V(H) \\ f(z) & z \in V^*(H) \end{cases}$$

Theorem

The matrix L_σ^H is invertible, and the solution to (4) is given by

$$u_2(z) = \begin{cases} \left((L_\sigma^H)^{-1} g\right)(z) & z \in V(H) \\ 0 & z \in V^*(H) \end{cases}$$

The matrix $(L_\sigma^H)^{-1}$ is a magnetic Green's function, in the sense that it is fundamental representation tool in the solution boundary value problem, both theoretically and in practice.

Result 2: Magnetic Green Identities

We develop two discrete Green's identities, which were funamental in the proofs of the preceding theorems. Let G, H be as in the previous result.

Theorem

Let $f, g \in \ell_2(V(\overline{H}))$. We have

$$\sum_{\{x,y\} \in E(\overline{H})} (f(x)\sigma_{xy} - f(y))\overline{(g(x)\sigma_{yx} - g(y))} - \sum_{x \in V(H)} f(x)\overline{\mathcal{L}_\sigma^{\overline{H}} g(x)} = \sum_{x \in V^*(H)} f(x)\overline{\frac{\partial g}{\partial \eta}(x)}$$

Theorem

Let $f, g \in \ell_2(V(\overline{H}))$. We have

$$\sum_{x \in V(H)} \mathcal{L}_\sigma^{\overline{H}} f(x)\overline{g(x)} - f(x)\overline{\mathcal{L}_\sigma^{\overline{H}} g(x)} = \sum_{x \in V^*(H)} f(x)\overline{\frac{\partial g}{\partial \eta}(x)} - \frac{\partial f}{\partial \eta}(x)\overline{g(x)}$$

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