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Letter to the Editor

Magnetic Eigenmaps for the visualization of directed networks

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ABSTRACT

We propose a framework for the visualization of directed networks relying on the eigenfunctions of the magnetic Laplacian, called here Magnetic Eigenmaps. The magnetic Laplacian is a complex deformation of the well-known combinatorial Laplacian. Features such as density of links and directionality patterns are revealed by plotting the phases of the first magnetic eigenvectors. An interpretation of the magnetic eigenvectors is given in connection with the angular synchronization problem. Illustrations of our method are given for both artificial and real networks.

1. Introduction

Many problems in neuroscience, biology, social or computer science are phrased in terms of networks and graphs. The embedding of data points forming undirected graphs can be performed using manifold learning methods, among which are the so-called Laplacian Eigenmaps [1] and Diffusion Maps [2]. In the same spirit, the embedding of a directed graph originating from the sampling of a vector field on a manifold was studied in [3]. A Laplacian for strongly connected and aperiodic directed networks was introduced by Chung [4] in relation with a random walk process, which was used for visualization e.g. in [5]. Actually, Laplacians are very useful tools for community detection and data visualization. A common feature of these approaches is the relevance of the discrete or combinatorial Laplacian, and its normalized versions. In the same context of directed graphs, an interesting approach for representing functions in terms of an orthogonal system was put forward very recently under general assumptions [6].

In this letter, no assumption on the origin of directed networks is needed, so we could deal, for example, with networks of webpages which are not embedded in any vector space. In particular, we propose here the use of another Laplacian which naturally exists for a general connected directed network, called the magnetic Laplacian. This operator is actually a vector bundle Laplacian as described in [7,8] and a Connection

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Laplacian [9]. Interestingly, the magnetic Laplacian can be interpreted as a discrete quantum mechanical Hamiltonian of a charged particle on a network, influenced by a magnetic flux [10–12]. The method that we describe assigns a complex rotation, i.e., an element of U(1), to each directed link, and the orientation of the link determines the direction of the rotation [13].

This letter is organized as follows. In Section 2 the magnetic Laplacian and its eigenvectors are introduced. A method using the complex phase of these eigenvectors for visualizing directed graphs is proposed in Section 3. Some examples are shown in Section 4, and the letter ends with some conclusions in Section 5.

2. Magnetic Laplacian and Eigenmaps

Consider a connected graph $\mathcal{G} = (V, E)$ with a set of N nodes V and a set of undirected edges E. In the case of an undirected graph, a symmetric weight matrix $W^{(\mathrm{s})}$ is given with elements $[W^{(\mathrm{s})}]_{ij} = w^{(\mathrm{s})}_{ij} \geq 0$ for all i and $j \in V$. The Laplacian Eigenmaps are the eigenvectors of the combinatorial Laplacian $L^{(0)} = D - W^{(\mathrm{s})}$, where D is the diagonal degree matrix with matrix elements $[D]_{ii} = d_i = \sum_{j\in V} w^{(\mathrm{s})}_{ij}$ for all $i \in V$. The volume of a subgraph $\mathcal{S}_A$ of $\mathcal{G}$ with node set A is simply $\mathrm{vol}(\mathcal{S}_A) = \sum_{i\in A} d_i$. In the case of directed networks, the graph is given by an asymmetric weight matrix W with elements $[W]_{ij} = w_{ij} \geq 0$. For simplicity, the weights are chosen to be binary, i.e., $w_{ij} = 1$ if there is a link from i to j and $w_{ij} = 0$ otherwise. The weight matrix W can be decomposed into a symmetric term $w^{(\mathrm{s})}_{ij} = (w_{ij} + w_{ji})/2$, indicating that $\{i, j\} \in E$, and a skew-symmetric term, the edge flow $a_{ij} = -a_{ji}$ encoding the direction of the link. For all $\{i, j\} \in E$, we have $a_{ij} = 1$ if the link points from i to j, and $a_{ij} = 0$ if $\{i, j\}$ is not directed.

In this letter, the magnetic Laplacian is defined as the self-adjoint, positive semi-definite operator $L^{(g)} = D - T^{(g)} \odot W^{(\mathrm{s})}$, where D is the degree matrix associated with the symmetrized weight matrix, $0 \leq g < 1/2$ is an electric charge parameter, and $[T^{(g)} \odot W^{(\mathrm{s})}]_{ij} = \exp(\mathrm{i}2\pi g a_{ji})\, w^{(\mathrm{s})}_{ij}$ (notice the Hadamard product $\odot$). The solutions of the generalized eigenvalue problem $L^{(g)}\phi = \lambda D\phi$ are the *Magnetic Eigenmaps* $\phi^{(g)}_k$ associated with the eigenvalues $\lambda^{(g)}_k \geq 0$ for $k \in \{0, \ldots, N-1\}$ [14] (we assume $\lambda^{(g)}_0 \leq \lambda^{(g)}_1 \leq \cdots \leq \lambda^{(g)}_{N-1}$).

2.1. Interpretation of the first eigenvectors

While the calculation of the *second* eigenvector of the normalized combinatorial Laplacian is a relaxation of the (normalized) cut problem, the calculation of the *first* eigenvector of the normalized magnetic Laplacian is a relaxation of the angular synchronization problem [15]. Given a subgraph $\mathcal{S}$ of $\mathcal{G}$ (in general, one can choose $\mathcal{S} = \mathcal{G}$), the angular synchronization problem consists in finding the angles $\boldsymbol{\theta}^\star = (\theta^\star_1, \ldots, \theta^\star_N)^\intercal \in \mathrm{U}(1)^N$ given by $\boldsymbol{\theta}^\star \in \arg\min_{\boldsymbol{\theta}}\ \eta_{\mathcal{S}}(\boldsymbol{\theta})$ where the frustration [16] is defined by

$$\eta_{\mathcal{S}}(\boldsymbol{\theta}) = \frac{1}{2}\frac{\sum_{i,j\in\mathcal{S}} w^{(\mathrm{s})}_{ij} |e^{\mathrm{i}\theta_i} - e^{\mathrm{i}\theta_{ij}} e^{\mathrm{i}\theta_j}|^2}{\sum_{i\in V} d_i},$$

with $\theta_{ij} = 2\pi g a_{ji}$ for all $i, j \in \mathcal{S}$ such that $w^{(\mathrm{s})}_{ij} \neq 0$. Notice that $\sum_{i\in V} d_i = \mathrm{vol}(\mathcal{G})$. The lowest eigenvector of the normalized magnetic Laplacian $\phi^{(g)}_0$ is the solution of the spectral problem relaxing $\min_{\boldsymbol{\theta}}\ \eta_{\mathcal{G}}(\boldsymbol{\theta})$. Our first conclusion is that computing the complex phase of $\phi^{(g)}_0$ yields an approximation of $\boldsymbol{\theta}^\star$ that we propose to choose as the first visualization coordinate. In [13], the solution of the angular synchronization problem is shown to provide a ranking of the nodes in directed graphs, although a slightly different eigenvector problem is considered.

The performance of the spectral relaxation of the cut problem can be studied using a classical result of spectral graph theory, the Cheeger inequality, which relates the Cheeger constant to the *second* smallest eigenvalue of the combinatorial Laplacian, providing the worst case performance for the spectral clustering method. Analogous results relate the *first* smallest eigenvalue of the Connection Laplacian [16] and the