Applied Mathematics and Computation 261 (2015) 382–387

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Effect on normalized graph Laplacian spectrum by motif attachment and duplication

Ranjit Mehatari [a], Anirban Banerjee [a,b,*]

[a] Department of Mathematics and Statistics, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India
[b] Department of Biological Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India

A R T I C L E I N F O

MSC:
05C75
47A75

Keywords:
Normalized graph Laplacian
Graph spectrum
Eigenvalue 1
Motif doubling
Motif attachment

A B S T R A C T

To some extent, graph evolutionary mechanisms can be explained by its spectra. Here, we are interested in two graph operations, namely, motif (subgraph) doubling and attachment that are biologically relevant. We investigate how these two processes affect the spectrum of the normalized graph Laplacian. A high (algebraic) multiplicity of the eigenvalues $1, 1 \pm 0.5, 1 \pm \sqrt{0.5}$ and others have been observed in the spectrum of many real networks. We attempt to explain the production of distinct eigenvalues by motif doubling and attachment. Results on the eigenvalue 1 are discussed separately.

1. Introduction

Nowadays, spectral graph theory is playing an important role to analyze the structure of real networks [2,4,10,14,17,22]. The underlying graph of biological and other real networks evolves with time. The evolutionary mechanisms may lead to the construction of certain local structures (motif) that could be described by different eigenvalues of normalized graph Laplacian [3,20]. Duplication of a group of genes [8,21] and horizontal [7,9] gene transfer may cause the existence of repetitive-motif and attachment of a distinct small network, respectively, in an existing biological network [15,18,19,21]. Two graph operations, motif doubling and attachment of a smaller graph into the existing graph, are interest of our study. Here we intensively investigate the emergence of particular eigenvalues such as eigenvalue 1 and other by the above-mentioned graph operations.

Let $\Gamma = (V, E)$ be a simple, connected, finite graph of order n with the vertex set V and the edge set E. Two vertices $i, j \in V(\Gamma)$, are connected by an edge in $E(\Gamma)$, are called neighbors, $i \sim j$. Let n_i be the degree of $i \in V(\Gamma)$, that is, the number of neighbors of i. For the function $g : V(\Gamma) \to \mathbb{R}$ we define the normalized graph Laplacian as

$$\Delta g(x) := g(x) - \frac{1}{n_x} \sum_{y, y \sim x} g(y). \qquad (1)$$

Note that, this operator is different from the (algebraic) graph Laplacian operator, $Lg(x) \coloneqq n_x g(x) - \sum_{y,\, y\,\sim\, x} g(y)$ (see [11,13,16] for this operator), but is similar to the Laplacian, $\mathcal{L}g(x) := g(x) - \sum_{y,y\sim x} \frac{1}{\sqrt{n_x n_y}} g(y)$ investigated in [6] and thus, both have the same spectrum. Now we recall some of the basic properties of eigenvalues and eigenfunctions of the operator (1) from [1]. The normalized Laplacian is symmetric for the product,

$$(g_1, g_2) := \sum_{i \in V} n_i g_1(i) g_2(i), \qquad (2)$$

* Corresponding author. Tel.: +91 9775320480; fax: +91 3325873020.
E-mail addresses: ranjit1224@iiserkol.ac.in (R. Mehatari), anirban.banerjee@iiserkol.ac.in (A. Banerjee).

http://dx.doi.org/10.1016/j.amc.2015.03.118

for real valued functions g_1, g_2 on $V(\Gamma)$. Since $(\Delta g, g) \geq 0$, all eigenvalues of Δ are non-negative. The eigenvalue equation of Δ is

$$\Delta f - \lambda f = 0, \tag{3}$$

where a non zero solution f is called an eigenfunction corresponding to the eigenvalue λ. If we arrange all the eigenvalues in a non-decreasing manner we have, $\lambda_0 = 0 < \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$, with $\lambda_{n-1} = 2$ *iff* the graph is bipartite. For a connected graph, the smallest eigenvalue is $\lambda_0 = 0$ with a constant eigenfunction. Since all the eigenfunctions are orthogonal to each other, for any eigenfunction f, we have

$$\sum_{i \in V} n_i f(i) = 0. \tag{4}$$

For a graph with N vertices, $\lambda_1 \leq \frac{N}{N-1} \leq \lambda_{N-1}$ and the equality hold *iff* the graph is complete, that is, for a complete graph $\lambda_1 = \lambda_2 = \cdots = \lambda_{N-1} = \frac{N}{N-1}$. Let m_λ be the algebraic multiplicity of the eigenvalues λ. The eigenvalue Eq. (3) becomes

$$\frac{1}{n_i} \sum_{j \sim i} f(j) = (1 - \lambda) f(i) \; \forall i \in \Gamma. \tag{5}$$

In particular, if an eigenfunction f vanishes at i, then $\Sigma_{j \sim i} f(j) = 0$, and conversely (for eigenvalue 1, the converse is not always true). For $\lambda = 1$, Eq. (5) becomes

$$\sum_{j \in \Gamma, j \sim i} f(j) = 0 \; \forall i \in \Gamma, \tag{6}$$

which is a special property of an eigenfunction for the eigenvalue 1. Note that, the nullity of the adjacency matrix [5] A of Γ is the same as the algebraic multiplicity of eigenvalue 1 in Δ. That is,

$$m_1 = \textit{nullity of } A. \tag{7}$$

The nullity of the adjacency matrix was very much studied in earlier mathematical works (see the survey by Gutman and Borovićanin [12]). Here, we take a different approach to study the eigenvalue 1 in the context of normalized graph Laplacian.

Now, we extend the discussion on the production of the eigenvalue 1 investigated in [1] and generalize the results to a broad range of operations.

Vertex doubling

Doubling of a vertex p of Γ is to add a vertex q to Γ and connect it to all j in Γ, whenever $j \sim p$. Vertex doubling, of a vertex p of Γ, ensures the eigenvalue 1 with an eigenfunction f_1 that takes value 1 at p, -1 at its double and 0 otherwise [1]. Now, if we double the vertex p, m times, then the resultant graph possesses the eigenvalue 1 with the multiplicity at least m with the corresponding eigenfunctions,

$$f_j^{(i)}(x) = \begin{cases} 1 & \text{if } x = p, q_1, q_2, \ldots, q_{j-1} \\ -j & \text{if } x = q_j \\ 0 & \text{else,} \end{cases} \tag{8}$$

for $j = 1, 2, \ldots, i$ and $i = 1, 2, \ldots, m$; where $q_1, q_2, q_3, \ldots, q_m$ are the vertices produced by repeated-doubling of p.

Motif doubling

Let Σ be a connected induced subgraph of Γ with vertices $p_1, \ldots, p_m$. Let Γ^Σ be obtained from Γ by adding a copy of the motif Σ consisting of the vertices $q_1, \ldots, q_m$ and the corresponding connections between them, and connecting each q_α with all $p \notin \Sigma$ that are neighbors of p_α. Now, if Σ has an eigenvalue 1 with an eigenfunction f_1^Σ, then Γ^Σ also ensures an eigenvalue 1 with the eigenfunction

$$f_1^{\Gamma^\Sigma}(p) = \begin{cases} f_1^\Sigma(p_\alpha) & \text{if } p = p_\alpha \in \Sigma \\ -f_1^\Sigma(p_\alpha) & \text{if } p = q_\alpha \\ 0 & \text{else,} \end{cases} \tag{9}$$

where q_α is the double of $p_\alpha \in \Sigma$ [1]. Now the above operation can easily be extendable for doubling Σ repeatedly m times. Let $\Sigma^1, \Sigma^2, \ldots, \Sigma^m$ be the doubles of Σ and the resultant graph is Γ^{Σ^m}, where $q_\alpha^{(m)} \in \Sigma^m$ is the double of p_α.

Theorem 1.1. *If Σ has an eigenvalue 1 with an eigenfunction f_1^Σ, then Γ^{Σ^m} also ensures an eigenvalue 1 with multiplicity at least m.*

Proof. For each $j = 1, 2, \ldots, m$ we have the eigenfunctions

$$f_j^{\Gamma^{\Sigma^m}}(p) = \begin{cases} f_1^\Sigma(p_\alpha) & \text{if } p = p_\alpha \in \Sigma \\ f_1^\Sigma(p_\alpha) & \text{if } p = q_\alpha^{(l)}, \quad j > 1, 1 \leq l \leq j-1 \\ -j f_1^\Sigma(p_\alpha) & \text{if } p = q_\alpha^{(j)} \\ 0 & \text{elsewhere,} \end{cases} \tag{10}$$

corresponding to eigenvalue 1. □