

Effect on normalized graph Laplacian spectrum by motif attachment and duplication

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Abstract

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 has 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.

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1 Introduction

Nowadays, spectral graph theory is playing an important role to analyze the structure of real networks [2, 4, 13, 17, 20, 25]. 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, 23]. Duplication of a group of genes [11, 24] and horizontal [9, 12] gene transfer may cause the existence of repetitive-motif and attachment of a distinct small network, respectively, in an existing biological network [18, 21, 22, 24]. 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 $g : V(\Gamma) \rightarrow \mathbb{R}$ we define the normalized graph Laplacian as

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

Note that, this operator is different from the (algebraic) graph Laplacian operator, $Lg(x) := n_x g(x) - \sum_{y, y \sim x} g(y)$ (see [14, 16, 19] 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 [8] 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,

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

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

$$\Delta f - \lambda f = 0, \quad (3)$$

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, $\lambda_0 = 0 < \lambda_1 \leq \dots \leq \lambda_{n-1} \leq 2$, 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

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

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 $\lambda_1 = \lambda_2 = \dots = \lambda_{N-1} = \frac{N}{N-1}$. Let m_λ be the algebraic multiplicity of the eigenvalues λ . The eigenvalue equation (3) becomes

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

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

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

which is a special property of an eigenfunction for the eigenvalue 1. Note that, the nullity of the adjacency matrix [7] A of Γ is the same as the algebraic multiplicity of eigenvalue 1 in Δ . That is,

$$m_1 = \text{nullity of } A. \quad (7)$$

The nullity of the adjacency matrix was very much studied in earlier mathematical Works (see the survey by Gutman and Borovićanin [15]) 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,

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

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

Motif Doubling:

Let Σ be a connected induced subgraph of Γ with vertices p_1, \dots, p_m . Let Γ^Σ be obtained from Γ by adding a copy of the motif Σ consisting of the vertices q_1, \dots, 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

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

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 $\Sigma^1, \Sigma^2, \dots, \Sigma^m$ 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 $j = 1, 2, \dots, m$ we have the eigenfunctions

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

corresponding to eigenvalue 1. □

Graph Attachment:

Let Γ_1 be a graph with an eigenfunction $f_1^{\Gamma_1}$ corresponding to an eigenvalue 1. We take a vertex $q \in \Gamma$ and another vertex $p \in \Gamma_1$ and construct $\Gamma_0 = \Gamma \cup \Gamma_1$ in such a way that Γ_0 contains all the connections of Γ and Γ_1 and in addition, we add edges from q to $j \in \Gamma_1$, whenever $j \sim p$.

Theorem 1.2. *Γ_0 possesses the eigenvalue 1 with an eigenfunction $f_1^{\Gamma_0}$.*

Proof. We choose

$$f_1^{\Gamma_0}(i) = \begin{cases} f_1^{\Gamma_1}(i) & \text{if } i \in \Gamma_1 \\ 0 & \text{if } i \in \Gamma. \end{cases} \quad (11)$$

□

Example: Let Γ be a triangle and Γ_1 be a chain of three vertices. Unlike Γ , Γ_1 has an eigenvalue 1. Now, we join any vertex from Γ to the both end vertices of Γ_1 and produce Γ_0 that possesses eigenvalue 1. Note that, if $m_1 = l$ in Γ_1 , Γ_0 ensures the eigenvalue 1 with the multiplicity at least l .

2 Eigenvalue λ

In this section, we describe how the graph operations, motif doubling and attachment of another graph produce a particular eigenvalue λ .

Motif Doubling :

Let Σ be a motif in Γ . Suppose a real valued function f satisfies

$$\frac{1}{n_i} \sum_{j \in \Sigma, j \sim i} f(j) = (1 - \lambda)f(i) \text{ for all } i \in \Sigma \text{ and some real value } \lambda, \quad (12)$$

where n_i is the degree of i in Γ . Let Γ^Σ be the graph obtained from Γ by doubling Σ in Γ [1]. Then Γ^Σ ensures an eigenvalue λ with the eigenfunction

$$f_\lambda^{\Gamma^\Sigma}(p) = \begin{cases} f(p_\alpha) & \text{if } p = p_\alpha \in \Sigma \\ -f(p_\alpha) & \text{if } p = q_\alpha, \\ 0 & \text{else.} \end{cases} \quad (13)$$

Theorem 2.1. Σ , is a motif in a graph Γ , consists of the vertices p_1, p_2, \dots, p_m . If Γ^Σ is obtained by doubling Σ in Γ , then the additional eigenvalues of the graph Γ^Σ are given by $A_\Sigma + (\lambda - 1)D_\Sigma = 0$, where A_Σ is the adjacency matrix of Σ and D_Σ is the diagonal matrix with the degrees of p_1, p_2, \dots, p_m .

Proof. From the eigenvalue equation (12) we get,

$$(\lambda - 1)f(p_i) + \sum_{p_j \in \Sigma, p_j \sim p_i} f(p_j) = 0, \quad \forall p_i \in \Sigma, \quad (14)$$

which gives a set of m homogeneous linear equations that can be written as:

$$AF = O, \quad (15)$$

where $A = A_\Sigma + (\lambda - 1)D_\Sigma$, $F = (f(p_1) \ f(p_2) \ \dots \ f(p_m))^T$ and $O = (0 \ 0 \ \dots \ 0)^T$. Now, to get a nonzero solution for f , we have

$$\det(A) = 0. \quad (16)$$

Hence the proof.

□

Example: Let Γ be a graph with more than three vertices and Σ be a chain, with the vertices, $p_1 - p_2 - p_3$. Now, from the theorem 2.1 we have

$$\begin{vmatrix} n_{p_1}(\lambda - 1) & 1 & 0 \\ 1 & n_{p_2}(\lambda - 1) & 1 \\ 0 & 1 & n_{p_3}(\lambda - 1) \end{vmatrix} = 0,$$

which gives $\lambda = 1, 1 \pm \sqrt{\frac{n_{p_1} + n_{p_3}}{n_{p_1} n_{p_2} n_{p_3}}}$. Note that, if $n_{p_1} = n_{p_2} = n_{p_3} = k$, then $\lambda = 1, 1 \pm \frac{\sqrt{2}}{k}$, that is, $\lambda \approx 1$ when k is very large.

Repeated Duplication of a Motif

The repeated doubling of a motif increases the multiplicity of the eigenvalue λ .

Theorem 2.2. *Let Σ , consists of the vertices p_1, p_2, \dots, p_m , be a motif in Γ . Suppose a nonzero real valued function f satisfies the equation*

$$\frac{1}{n_{p_i}} \sum_{p_j \in \Sigma, p_j \sim p_i} f(p_j) = (1 - \lambda)f(p_i), \text{ for all } p_i \in \Sigma \text{ and some real value } \lambda, \quad (17)$$

where n_{p_i} is the degree of the vertex p_i in Γ . If Γ^{Σ^m} is the graph obtained from Γ by repeatedly doubling Σ m times, as we described in theorem 1.1, then Γ^{Σ^m} ensures the eigenvalue λ with the multiplicity at least m .

Proof. We construct m eigenfunctions:

$$f_j^{\Gamma^{\Sigma^m}}(p) = \begin{cases} f(p_\alpha) & \text{if } p = p_\alpha \in \Sigma \\ f(p_\alpha) & \text{if } p = q_\alpha^{(l)}, j > 1, 1 \leq l \leq j - 1 \\ -j f(p_\alpha) & \text{if } p = q_\alpha^{(j)} \\ 0 & \text{else} \end{cases} \quad (18)$$

$j = 1, 2, \dots, m$ corresponding to the eigenvalue λ , in Γ^{Σ^m} . □

Example (star of triangles): Let Γ^i denotes the star with i triangles, that is, i triangles are joined at a single vertex. Theorem 2.1 and theorem 2.2 show that the eigenvalues of Γ^i are 0, 0.5 and 1.5 with multiplicities 1, $i - 1$ and $i + 1$ respectively, whereas the theorem 2.2 provides the corresponding eigenfunctions.

Graph Attachment :

Now, we discuss about the production of an particular eigenvalue λ due to graph attachment, that is, we add a graph Σ to an existing graph Γ (the spectrum of algebraic graph Laplacian produced by a particular graph attachment operation has been discussed in [19]). Here, the attachment operation is different than what we described in section (1). Let Σ_c be an induced subgraph of Σ . We take a vertex $p \in \Gamma$ and join p to all $j \in \Sigma_c$ by an edge and get the resultant graph Γ^Σ . Now, we have the following theorem associated to this operation.

Theorem 2.3. *If there exists a nonzero real valued function f which satisfies the equation*

$$\frac{1}{n_i} \sum_{j \in \Sigma, j \sim i} f(j) = (1 - \lambda)f(i), \text{ for all } i \in \Sigma \text{ and some real value } \lambda \quad (19)$$

and

$$\sum_{j \in \Sigma_c} f(j) = 0, \quad (20)$$

where n_i is the degree of i in Γ^Σ , then Γ^Σ possesses the eigenvalue λ with an eigenfunction f^{Γ^Σ} which coincides with f on Σ .

Proof. We take,

$$f^{\Gamma^\Sigma}(p) = \begin{cases} f(p) & \text{if } p \in \Sigma \\ 0 & \text{otherwise.} \end{cases}$$

□

Corollary 2.1. *Let Σ be a regular graph. We join a vertex $p \in \Gamma$ to all the vertices in Σ and get a new graph Γ^Σ . Now, if there exists a nonzero real valued function f which satisfies the equation $\frac{1}{n_i} \sum_{j \in \Sigma, j \sim i} f(j) = (1 - \lambda)f(i)$, for all $i \in \Sigma$ and some real value λ (where n_i is the degree of i in Γ^Σ), then Γ^Σ possesses the eigenvalue λ with the eigenfunction f^{Γ^Σ} which coincides with f on Σ .*

Proof. Here $\Sigma_c = \Sigma$ and $\langle f^{\Gamma^\Sigma}, f_0 \rangle = 0$, where f_0 is a constant eigenfunction. □

Corollary 2.2. *The above corollary 2.1 also holds if Σ is the complete graph K_n . Moreover, here $\lambda = \frac{n+1}{n}$ with $m_\lambda = n - 1$.*

Proof. Since a complete graph is regular, the first part of the corollary follows from the corollary 2.1. Now, if we consider the graph $\Sigma' = \Sigma \cup \{p\}$ obtained by taking all the edges of Σ and the edges (i, p) for all $i \in \Sigma$, then Σ' becomes K_{n+1} that has the eigenvalue $\lambda = \frac{n+1}{n}$ with $n - 1$ eigenfunctions f_λ^i , $i = 1, 2, \dots, n - 1$ which takes the value 0 at p , and $\sum_{j \in \Sigma} f_\lambda^i(j) = 0$ for $i = 1, 2, \dots, n - 1$. Thus, each f_λ^i can be extended to an eigenfunction of Γ^Σ . Hence the proof. □

Example: If we consider Γ and Σ both to be K_2 , then by the above corollary we get $\lambda = 1.5$ with an eigenfunction $f_{1.5} = [0 \ 0 \ 1 \ -1]^T$.

Example (Kite $K(m, n)$): A kite $K(m, n)$ is a graph with $m+n+1$ vertices obtained by joining all the vertices of K_m and K_n to a single vertex α . Thus $K(m, n)$ has m vertices, p_1, \dots, p_m , with degree m , n vertices q_1, \dots, q_n , with degree n , and a vertex α of degree $m+n$. Thus, $K(m, n) - \alpha = K_m \cup K_n$. Now, the corollary 2.2 shows that $K(m, n)$ has eigenvalues $\frac{m+1}{m}$ and $\frac{n+1}{n}$ with the multiplicity $m - 1$ and $n - 1$ respectively. The rest two eigenvalues are λ_β and λ_γ , such that, $\lambda_\beta + \lambda_\gamma = 1 + \frac{1}{m} + \frac{1}{n}$. Note that, using theorem 2.1 we get $K(m, m)$ has the eigenvalues 0, $\frac{m+1}{m}$ and $\frac{1}{m}$ with the multiplicity 1, $2m - 1$, and 1 respectively.

Corollary 2.3. *If we join all vertices of Σ to the vertices $p_1, p_2, \dots, p_k \in \Gamma$, then the theorem 2.3 also holds trivially.*

Proof. We take the eigenfunction

$$f^{\Gamma^\Sigma}(p) = \begin{cases} f(p) & \text{if } p \in \Sigma \\ 0 & \text{otherwise} \end{cases}$$

corresponding to the eigenvalue λ . \square

Corollary 2.4. *Now we combine corollary 2.2 and corollary 2.3, that is, we take Σ to be K_n and we obtain Γ^Σ by joining all vertices Σ to the vertices $p_1, p_2, \dots, p_k \in \Gamma$. Now, the resultant graph posses the eigenvalue $\lambda = \frac{n+k}{n+k-1}$ with $m_\lambda = n - 1$.*

Proof. The proof is similar in corollary 2.2. Here $\Sigma' = \Sigma \cup \{p_1, p_2, \dots, p_k\}$ obtained by taking all the edges of Σ and the edges (i, p_j) , for all $i \in \Sigma$ and $j = 1, 2, \dots, k$. Thus the Σ' becomes K_{n+k} which has the eigenvalue $\lambda = \frac{n+k}{n+k-1}$ with $n - 1$ eigenfunctions f_λ^i , $i = 1, 2, \dots, n - 1$ that take the value 0 at p_1, p_2, \dots, p_k , and $\sum_{j \in \Sigma} f_\lambda^i(j) = 0$ for $i = 1, 2, \dots, n - 1$. Since $f_\lambda^i(p_j) = 0$ for $j = 1, 2, \dots, k$, every f_λ^i can be extended to an eigenfunction of Γ^Σ for $i = 1, 2, \dots, n - 1$. \square

Note that, if we delete any edge (p_l, p_j) in corollary 2.4, λ becomes unchanged. Now, we generalize the fact in the theorem 2.3. Let $\Sigma_{c_1}, \Sigma_{c_2}, \dots, \Sigma_{c_k}$ be induced subgraphs (not necessarily having disjoint vertex sets) of Σ . We take distinct vertices $p_1, p_2, \dots, p_k \in \Gamma$ and join all vertices $j \in \Sigma_{c_l}$ by an edge to p_l , for all $l = 1, 2, \dots, k$ and produce Γ^Σ .

Theorem 2.4. *If there exists a nonzero real valued function f which satisfies*

$$\frac{1}{n_i} \sum_{j \in \Sigma, j \sim i} f(j) = (1 - \lambda)f(i) \text{ for all } i \in \Sigma \text{ and some real value } \lambda \quad (21)$$

and

$$\sum_{j \in \Sigma_{c_l}} f(j) = 0 \text{ for } l = 1, 2, \dots, k, \quad (22)$$

where n_i is the degree of i in Γ^Σ , then Γ^Σ possesses the eigenvalue λ with an eigenfunction f^{Γ^Σ} which coincides with f on Σ .

Proof. We construct the eigenfunction

$$f^{\Gamma^\Sigma}(p) = \begin{cases} f(p) & \text{if } p \in \Sigma \\ 0 & \text{otherwise.} \end{cases}$$

\square

Now, we take both Γ and Σ are regular. Let us consider $V(\Gamma) = \{p_1, p_2, \dots, p_n\}$, $V(\Sigma) = \bigcup_{i=1}^n V(\Sigma_{c_i})$ with $|V(\Sigma_{c_i})| = |V(\Sigma_{c_j})| \forall i, j$ and $|\{\Sigma_{c_i} : x \in \Sigma_{c_i}\}| = k$ (constant) $\forall x \in \Sigma$. Let Γ^Σ be the graph obtained by joining all vertices of Σ_{c_i} to p_i . Thus $\{\Gamma, \Sigma\}$ becomes an equitable partition of Γ^Σ . Now, the statement of the theorem 2.4 changes for this construction and follows as:

Corollary 2.5. *If Σ be r -regular, then a nonzero real valued function f , which satisfies $\frac{1}{r+k} \sum_{j \in \Sigma, j \sim i} f(j) = (1 - \lambda)f(i)$, for all $i \in \Sigma$ and some real value λ and $\sum_{j \in \Sigma_{c_l}} f(j) = 0$, for $l = 1, 2, \dots, n$, can be extended to an eigenfunction corresponding to the eigenvalue λ for the graph Γ^Σ .*

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