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On the spectrum of the normalized graph Laplacian

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Abstract

We investigate how the spectrum of the normalized (geometric) graph Laplacian is affected by operations like motif dougling, graph splitting or joining. The multiplicity of the eigenvalue 1, or equivalently, the dimension of the kernel of the adjacency matrix of the graph is of particular interest. This multiplicity can be increased, for instance, by motif doubling.

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0. Introduction

Let Γ be a finite and connected graph with N vertices. Two vertices $i, j \in \Gamma$ are called neighbors, $i \sim j$, when they are connected by an edge of Γ. For a vertex $i \in \Gamma$, let n_i be its degree, that is, the number of its neighbors. For functions v from the vertices of Γ to $\mathbb{R}$, we define the (normalized) Laplacian as

$$\Delta v(i) := v(i) - \frac{1}{n_i} \sum_{j, j \sim i} v(j). \tag{1}$$

This is different from the operator $Lv(i) := n_i v(i) - \sum_{j, j\sim i} v(j)$ usually studied in the graph theoretical literature as the (algebraic) graph Laplacian, see e.g. [3,7,10,11,2], but equivalent to the

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Laplacian investigated in [4]. This normalized Laplacian is, for example, the operator underlying random walks on graphs, and in contrast to the algebraic Laplacian, it naturally incorporates a conservation law.

We are interested in the spectrum of this operator as yielding important invariants of the underlying graph Γ and incorporating its qualitative properties. As in the case of the algebraic Laplacian, one can essentially recover the graph from its spectrum, up to isospectral graphs. The latter are known to exist, but are relatively rare and qualitatively quite similar in most respects (see e.g. [12] for a systematic discussion). For a heuristic algorithm for the algebraic Laplacian which can be easily modified for the normalized Laplacian, see [8].

We now recall some elementary properties, see e.g. [4,9]. The normalized Laplacian, henceforth simply called the Laplacian, is symmetric for the product

$$(u, v) := \sum_{i \in V} n_i u(i) v(i) \tag{2}$$

for real valued functions u, v on the vertices of Γ. Δ is nonnegative in the sense that $(\Delta u, u) \geqslant 0$ for all u.

From these properties, we conclude that the eigenvalues of Δ are real and nonnegative, where the eigenvalue equation is

$$\Delta u - \lambda u = 0. \tag{3}$$

A nonzero solution u is called an eigenfunction for the eigenvalue λ.

The smallest eigenvalue is $\lambda_0 = 0$, with a constant eigenfunction. Since we assume that Γ is connected, this eigenvalue is simple, that is

$$\lambda_k > 0 \tag{4}$$

for $k > 0$ where we order the eigenvalues as

$$\begin{aligned} &\lambda_0 = 0 < \lambda_1 \leqslant \cdots \leqslant \lambda_{N-1}, \\ &\lambda_{N-1} \leqslant 2 \end{aligned} \tag{5}$$

with equality iff the graph is bipartite. The latter is also equivalent to the fact that whenever λ is an eigenvalue, then so is $2 - \lambda$.

For a complete graph of N vertices, we have

$$\lambda_1 = \cdots = \lambda_{N-1} = \frac{N}{N-1}, \tag{6}$$

that is, the eigenvalue $\frac{N}{N-1}$ occurs with multiplicity $N - 1$. Among all graphs with N vertices, this is the largest possible value for λ_1 and the smallest possible value for λ_{N-1}.

The eigenvalue equation (3) is

$$\frac{1}{n_i} \sum_{j \sim i} u(j) = (1 - \lambda) u(i) \quad \text{for all } i. \tag{7}$$

In particular, when the eigenfunction u vanishes at i, then also $\sum_{j \sim i} u(j) = 0$, and conversely (except for $\lambda = 1$). This observation will be useful for us below.

1. The eigenvalue 1

For the eigenvalue $\lambda = 1$, Eq. (7) becomes simply

$$\sum_{j\sim i} u(j) = 0 \quad \text{for all } i, \tag{8}$$

that is, the average of the neighboring values vanishes for each i. We call a solution u of (8) balanced. The multiplicity m_1 of the eigenvalue 1 then equals the number of linearly independent balanced functions on Γ.

There is an equivalent algebraic formulation: Let $A = (a_{ij})$ be the adjacency matrix of Γ; $a_{ij} = 1$ if i and j are connected by an edge and =0 else. Eq. (8) then simply means

$$Au = \sum_j a_{ij} u(j) = 0, \tag{9}$$

that is, the vector $u(j)_{j\in\Gamma}$ is in the kernel of the adjacency matrix. Thus,

$$m_1 = \dim\ker A. \tag{10}$$

We are interested in the question of estimating the multiplicity of the eigenvalue 1 on a graph. An obvious method for this is to determine restrictions on corresponding eigenfunctions f_1. We shall do that by graph theoretical considerations, and in this sense, this constitutes a geometric approach to the algebraic question of determining or estimating the kernel of a symmetric 0–1 matrix with vanishing diagonal. Bevis et al. [1] systematically investigated the effect of the addition of a single vertex on m_1. Here, we are also interested in the effect of more global graph operations.

We start with the following simple observation:

Lemma 1.1. *Let q be a vertex of degree 1 in Γ (such a q is called a pending vertex). Then any eigenfunction f_1 for the eigenvalue 1 vanishes at the unique neighbor of q.*

2. Motif doubling, graph splitting and joining

Let Σ be a connected subgraph of Γ with vertices $p_1, \ldots, p_m$, containing all of Γ's edges between those vertices. We call such a Σ a motif. The situation we have in mind is where N, the number of vertices of Γ, is large while m, the number of vertices of Σ, is small. Let 1 be an eigenvalue of Σ with eigenfunction f_1^Σ. f_1^Σ when extended by 0 outside Σ to all of Γ need not be an eigenfunction of Γ, and 1 need not even be an eigenvalue of Γ. We can, however, enlarge Γ by doubling the motif Σ so that the enlarged graph also possesses the eigenvalue 1, with a localized eigenfunction:

Theorem 2.1. *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. Then Γ^Σ possesses the eigenvalue 1, with a localized eigenfunction that is nonzero only at the p_α and the q_α.*

Proof. A corresponding eigenfunction is obtained as

$$f_1^{\Gamma^\Sigma}(p) = \begin{cases} f_1^\Sigma(p_\alpha) & \text{if } p = p_\alpha \in \Sigma, \\ -f_1^\Sigma(p_\alpha) & \text{if } p = q_\alpha, \\ 0 & \text{else.} \end{cases} \qquad \square \tag{11}$$

The theorem also holds for the case where Σ is a single vertex p_1 (even though such a motif does not possess the eigenvalue 1 itself). Thus, we can always produce the eigenvalue by *vertex doubling*. This is a reformulation of a result of [6].

Theorem 2.1, however, does not apply to eigenvalues other than 1 because for $\lambda \neq 1$, the vertex degrees n_i in (7) are important, and this is affected by embedding the motif Σ into another graph Γ. However, we have the following variant in the general case.

Theorem 2.2. *Let Σ be a motif in Γ. Suppose f satisfies*

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

Then the motif doubling of Theorem 2.1 produces a graph Γ^Σ with eigenvalue λ and an eigenfunction f^{Γ^Σ} agreeing with f on Σ, with $-f$ on the double of Σ, and being 0 on the rest of Γ^Σ.

Proof. Eq. (12) implies that f satisfies the eigenvalue equation on Σ, and therefore $-f$ satisfies it on its double. As before, the doubling has the effect that for all other vertices $j \in \Gamma^\Sigma$,

$$\frac{1}{n_j}\sum_{\ell\sim j} f^{\Gamma^\Sigma}(\ell) = 0. \qquad \square \tag{13}$$

The simplest motif is an edge connecting two vertices p_1, p_2. The corresponding relations (12) then are

$$\frac{1}{n_{p_1}} f(p_2) = (1-\lambda)f(p_1), \qquad \frac{1}{n_{p_2}} f(p_1) = (1-\lambda)f(p_2) \tag{14}$$

which admit the solutions

$$\lambda = 1 \pm \frac{1}{\sqrt{n_{p_1} n_{p_2}}}. \tag{15}$$

Thus edge doubling leads to those eigenvalues which when p_1 or p_2 has a large degree become close to 1. In any case, the two values are symmetric about 1.

We can also double the entire graph:

Theorem 2.3. *Let Γ_1 and Γ_2 be isomorphic graphs with vertices $p_1, \ldots, p_n$ and $q_1, \ldots, q_n$ respectively, where p_i corresponds to q_i, for $i = 1, \ldots, n$. We then construct a graph Γ_0 by connecting p_i with q_j whenever $p_j \sim p_i$. If $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of Γ_1 and Γ_2, then Γ_0 has these same eigenvalues, and the eigenvalue 1 with multiplicity n.*

Proof. Since the degree of every vertex p in Γ_0 is $2n_p$ where n_p is its original degree in Γ_1, we have for an eigenfunction f_λ of Γ_1 (which then is also an eigenfunction on Γ_2),

$$\frac{1}{2n_p}\sum_{s\in\Gamma_0, s\sim p} f_\lambda(s) = \frac{1}{n_p}\sum_{s\in\Gamma_1, s\sim p} f_\lambda(s) = (1-\lambda)f_\lambda(p). \tag{16}$$

Thus, by (7), it is an eigenfunction on Γ_0.

Finally, similarly to the proof of Theorem 2.1, we obtain the eigenvalue 1 with multiplicity n: for each $p \in \Gamma_1$, we construct an eigenfunction with value 1 at p, -1 at its double in Γ_2, and 0 elsewhere. $\square$

We now turn to a different operation. Let Γ be a graph with an eigenfunction f_1. We arbitrarily divide Γ into subgraphs $\Sigma_0, \Sigma_1, \Sigma_2$ such that there is no edge between an element of Σ_1 and an element of Σ_2. We then take the graphs $\Gamma_1 = \Sigma_1 \cup \Sigma_0$ and $\Gamma_2 = \Sigma_2 \cup \Sigma_0$, in such a manner that each edge between two elements of Σ_0 is contained in either Γ_1 or Γ_2, but not in both of them, and form a connected graph Γ_0 by taking an additional vertices w for each vertex $q \in \Sigma_0$ and connect it with the two copies of q in Γ_1 and Γ_2.

Theorem 2.4. *Γ_0 possesses the eigenvalue* 1 *with an eigenfunction that agrees with f_1 on Γ_1.*

Proof. We put

$$f_1^{\Gamma_0}(p) = \begin{cases} f_1(p) & \text{for } p \in \Gamma_1, \\ -f_1(p) & \text{for } p \in \Gamma_2, \\ -\sum_{s \in \Gamma_1, s \sim q} f_1(s) & \text{when } p = w \text{ is one of the added vertices} \\ & \text{connected to } q \in \Gamma_1. \end{cases} \tag{17}$$

This works out because $\sum_{s \in \Gamma_1, s\sim q} f_1(s) + \sum_{s \in \Gamma_2, s \sim q} f_1(s) = \sum_{s \in \Gamma, s\sim q} f_1(s) = 0$ since f_1 is an eigenfunction on Γ. □

A simple and special case consists in taking a node p and joining a chain of length 2 to it, that is, connect p with a new node p_1 and that node in turn with another new node p_2 and put the value 0 at p_1 and the value $-f_1(p)$ at p_2. This case was obtained in [1].

The next operation, graph joining, works for any eigenvalue, not just 1:

Theorem 2.5. *Let Γ_1, Γ_2 be graphs with the same eigenvalue λ and corresponding eigenfunctions f_λ^1, f_λ^2. Assume that $f_\lambda^1(p_1) = 0$ and $f_\lambda^2(p_2) = 0$ for some $p_1 \in \Gamma_1$, $p_2 \in \Gamma_2$. Then the graph Γ obtained by joining Γ_1 and Γ_2 via identifying p_1 with p_2 also has the eigenvalue λ with an eigenfunction given by f_λ^1 on Γ_1, f_λ^2 on Γ_2.*

Proof. We observe from (7) that for an eigenfunction f_λ whenever $f_\lambda(q) = 0$ at some q, then also $\sum_{s\sim q} f_\lambda(s) = 0$. This applies to p_1 and p_2, and therefore, we can also join the eigenfunctions on the two components. □

This includes the case where either f_λ^1 or f_λ^2 is identically 0.

Example. A triangle, that is, a complete graph of three vertices i_1, i_2, i_3, possesses the eigenvalue 3/2 with multiplicity 2. An eigenfunction $f_{3/2}$ vanishes at one of the vertices, say $f_{3/2}(i_1) = 0$ and takes the values +1 and -1, respectively, at the two other ones. Thus, when a triangle is joined at one vertex to another graph, the eigenvalue 3/2 is kept. For instance (see [4]), the petal graph, that is, a graph where m triangles are joined at a single vertex, has the eigenvalue 3/2 with multiplicity $m + 1$ (here, m of these eigenvalues are obtained via the described construction, and the remaining eigenfunction has the value -2 at the central vertex where all the triangles are joined and 1 at all other ones).

Also, when the condition of Theorem 2.5 is satisfied at several pairs of vertices, we can form more bonds by vertex identifications between the two graphs. For the eigenvalue 1, the situation is even better: We need not require $f_\lambda^1(p_1) = 0$ and $f_\lambda^2(p_2) = 0$, but only $f_\lambda^1(p_1) = f_\lambda^2(p_2)$ to make the joining construction work.

3. Examples

A chain of m vertices (that is, where we have an edge between p_j and p_{j+1} for $j = 1, \ldots, m-1$), by the lemma and node doubling, possesses the eigenvalue 1 (with multiplicity 1) iff m is odd, with eigenfunction $f_1(p_1) = 1$, $f_1(p_2) = 0$, $f_1(p_3) = -1$, $f_1(p_4) = 0, \ldots$ Similarly, a closed chain (that is, where we add an edge between p_m and p_1) possesses the eigenvalue 1 (with multiplicity 2) iff m is a multiple of 4.

Local operations like adding an edge may increase or decrease m_1 or leave it invariant. Adding a pending vertex to a chain of length 2 increases m_1 from 0 to 1, adding a pending vertex to closed chain of length 3, a triangle, leaves $m_1 = 0$, adding a pending vertex to a closed chain of length 4, a quadrangle, reduces m_1 from 2 to 1 (see [1] for general results in this direction). Similarly, closing a chain by adding an edge between the first and last vertex may increase, decrease or leave m_1 the same.

In any case, the question of the eigenvalue 1 is not a local one. Take closed chains of lengths $4k-1$ and $4\ell+1$. Neither of them supports the eigenvalue 1, but if we join them at a single point (that is, we take a point p_0 in the first and a point q_0 in the second graph and form a new graph by identifying p_0 and q_0), the resulting graph has 1 as an eigenvalue. An eigenfunction has the value 1 at the joined node, and the values ± 1 occurring always in neighboring pairs in the rest of the chains, where the two neighbors of p_0 in the first chain both get the value -1, and the ones in the second chain the value 1.

4. Construction of graphs with eigenvalue 1 from given data

Let f be an integer valued function on the vertices of the graph Γ. We define the excess of $p \in \Gamma$ as

$$e(p) := \sum_{q \sim p} f(q). \tag{18}$$

Thus, f is an eigenfunction for the eigenvalue 1 iff $e(p) = 0$ for all p.

We are going to show that we can construct graphs Γ and functions f with the property that $e(p) = 0$ except for one single vertex p_0 where the pair $(f(p), e(p))$ assumes any prescribed integer values (n, m). These will be assembled from elementary building blocks.

1. A triangle with a function f that takes the value -1 at two vertices and the value 1 at the third vertex, our p_0, realizes the pair $(1, -2)$.
2. The same triangle, with a pending vertex, our new p_0, connected to the vertex with value 1, and given the value 2, realizes $(2, 1)$.
3. Joining instead ℓ triangles at a single vertex, our p_0, with value 1, assigning -1 to all the other vertices as before, yields $(1, -2\ell)$.
4. A pentagon, i.e., a closed chain of five vertices, with value -1 at two adjacent vertices and 1 at the remaining three, the middle one of which is our p_0, realizes $(1, 2)$.
5. Similarly, adding a pending vertex, again our new p_0, connected to the former p_0 in the pentagon, and assigned the value -2, realizes $(-2, 1)$.
6. Likewise, joining ℓ such pentagons instead at p_0 yields $(1, 2\ell)$.
7. In general, connecting a pending vertex as the new p_0 to the former p_0 changes (n, m) to $(-m, n)$.
8. In general, joining the p_0s from graphs with values $(n, m_1), \ldots, (n, m_k)$ yields $(n, \sum_1^k m_j)$.

Thus, from the triangle and the pentagon, by adding pending vertices and graph joining, we can indeed realize all integer pairs (n, m).

Theorem 4.1. *Let Σ be a graph, f an integer valued function on its vertices. We can then construct a graph Γ containing the motif Σ with eigenvalue* 1 *and an eigenfunction coinciding with f on Σ.*

Proof. At each $p \in \Sigma$, we attach a graph realizing the pair $(f(p), -e(p))$. This ensures (7) at p. □

The preceding constructions also tell us how m_1, the multiplicity of the eigenvalue 1, behaves when we modify a graph Γ', consisting possibly of two disjoint components Γ_1, Γ_2, by either identifying vertices or by joining vertices by new edges. The graph resulting from these operations will be called Γ. We consider two cases:

1. We identify the vertex p_j with q_j for $j = 1, \ldots, m$, assuming that they do not have common neighbors. Then
   (a) We can generate an eigenfunction on Γ whenever we find a function g on Γ' with vanishing excess except possibly at the joined points where we require
   $$g(p_j) = g(q_j) \quad \text{and} \quad e_g(p_j) = -e_g(q_j) \quad \text{for } j = 1, \ldots, m. \tag{19}$$
   (b) As a special case of (19), an eigenfunction $f_1^{\Gamma'}$ produces an eigenfunction f_1^{Γ} whenever
   $$f_1^{\Gamma'}(p_j) = f_1^{\Gamma'}(q_j) \quad \text{for } j = 1, \ldots, m. \tag{20}$$
   In the case where Γ' consists of two disjoint components Γ_1, Γ_2, this includes the case where that value is 0 for all j and $f_1^{\Gamma'}$ vanishes identically on one of the components. In other words, we can extend an eigenfunction from Γ_1, say, to the rest of the graph by 0 whenever that function vanishes at all joining points.
   Since in general, Eq. (20) cannot be satisfied for a basis of eigenfunctions, by this process, we can only expect to generate fewer than $m_1^{\Gamma'}$ linearly independent eigenfunctions on Γ.

   Whether m_1^{Γ} is larger or smaller than $m_1^{\Gamma'}$ then depends on the balance between these two processes, that is, how many eigenfunctions satisfy (20) vs. how many new eigenfunctions can be produced by functions satisfying (19) with nonvanishing excess at some of the joined vertices.
2. We connect the vertex p_j by an edge with q_j for $j = 1, \ldots, m$. Then
   (a) We can generate eigenfunctions on Γ whenever we find a function g on Γ' with vanishing excess except possibly at the connected points where we require
   $$g(p_j) = -e_g(q_j) \quad \text{and} \quad g(q_j) = -e_g(p_j) \quad \text{for } j = 1, \ldots, m. \tag{21}$$
   (b) Again, as a special case of (21), an eigenfunctions $f_1^{\Gamma'}$ produces an eigenfunction f_1^{Γ} whenever
   $$f_1^{\Gamma'}(p_j) = 0 = f_1^{\Gamma'}(q_j) \quad \text{for } j = 1, \ldots, m. \tag{22}$$
   This imposes a stronger constraint than in (20) on eigenfunctions to yield an eigenfunction on Γ.

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