12

The Nonbacktracking Laplacian

A nonbacktracking random walk, that is, where the random walker is not allowed to travel an edge back and forth, leads to a new Laplace-type operator with novel properties. It encodes structural features of the underlying graph in a manner different from other Laplace operators.

Spectral graph theory is typically based on the study of the spectrum of symmetric operators associated with graphs. As discussed in Chapters 4, 5, and 8, the main advantage is that such spectra can be easily computed and are relatively easy to interpret in terms of geometric properties of the graph. The price to pay is the presence of several families of isospectral graphs, that is, nonisomorphic graphs that share the same spectrum and therefore cannot be uniquely distinguished by their eigenvalues.

An alternative to the spectral theory of graphs via symmetric operators, which partially overcomes this problem and also comes with its own interesting aspects, is the spectral theory of *nonbacktracking operators*. The idea behind it is the following. Consider a simple graph $G = (V, E)$ and a random walker on V who moves, with uniform probability, from one vertex v to any of its neighbors, except for the one that she visited immediately prior to v. This process is called a *nonbacktracking random walk* since the walker does not go back to the vertex she just visited, and it is clearly non-Markovian. However, it is possible to construct a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ called the *nonbacktracking graph* or the *Hashimoto graph* of G, with the property that a nonbacktracking random walk on V can be equivalently seen as a simple random walk on $\mathcal{V}$, and this process is Markovian on $\mathcal{V}$. We shall see how to construct $\mathcal{G}$ in the first section of this chapter.

The reader may have already noticed that we are deviating here from our general convention to denote a graph by Γ and call it G instead. The reason is that our notation in this chapter is set up so as to utilize a systematic correspondence between ordinary and calligraphic letters. The ordinary letters,

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like G, will be used for quantities defined on or by the original graph, and the calligraphic letters, $\mathcal{G}$ in this case, for the corresponding quantities on the nonbacktracking graph constructed from it. So, for instance, V is the vertex set of G and $\mathcal{V}$ that of $\mathcal{G}$. Also, in this chapter, it will be natural to work with *directed* graphs.

The adjacency matrix $\mathcal{A}$ and the normalized Laplacian $\mathcal{L}$ of the new directed graph $\mathcal{G}$ are nonsymmetric operators, and, as we shall see, their spectra can be considered in order to investigate properties of the original graph G. We recall the discussion of general non symmetric Laplacians in Section 4.7.

The transpose of $\mathcal{A}$ is called the *nonbacktracking matrix* of G, and it was introduced by Ki-ichiro Hashimoto in 1989 in the context of graph zeta functions [127]. Later on, many properties of this matrix have been investigated in the area of algebraic graph theory [22, 66, 257], and it has then been shown that it is very powerful in spectral graph theory, as well as in its applications to network analysis [8, 36, 67, 111, 116, 177, 202, 226, 259–262]. Moreover, Backhausz, Szegedy, and Virág applied nonbacktracking random walks to the study of Ramanujan graphings [13], while Shrestha, Scarpino, and Moore in 2015 [250], as well as Castellano and Pastor-Satorras in 2018 [48], applied the study of nonbacktracking paths to epidemic spreading on networks.

The matrix $\mathcal{L}$ is called the *nonbacktracking Laplacian* of G. It was introduced in [156] (on which this chapter is mainly based) and further investigated in [220].

Before proceeding, we should warn the reader that, once one learns about the beauty of the nonbacktracking matrices, there is no going back to only working with symmetric operators.

12.1 Basic Definitions

We now give a formal and detailed description of the concepts that we introduced at the beginning of this chapter.

We fix a simple graph $G = (V, E)$ on N nodes and M edges and (for reasons that will soon be clear) we assume that it has minimum degree ≥ 2. For each edge, we fix an *orientation*; that is, we let one of its endpoints be its *input* and the other one be its *output*. Moreover, we let $e = [v, w]$ denote the oriented edge whose input is v and whose output is w. We also write $\mathrm{in}(e) := v$ and $\mathrm{out}(e) := w$, and we let $e^{-1} := [w, v]$. We also let $e_1, \dots, e_M$ denote the edges of G with the orientation that has been (arbitrarily) fixed, and we let

$$e_{M+1} := e_1^{-1}, \dots, e_{2M} := e_M^{-1}$$

denote the edges with the inverse orientation.

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Earlier, we described a nonbacktracking random walk as a non-Markovian process on the vertex set of G. We can equivalently define it as a Markovian process on the set of oriented edges, as follows.

Definition 12.1.1. A *nonbacktracking random walk* on G is a discrete-time Markov process on the oriented edges such that the probability of going from e_i to e_j is

$$\mathbb{P}(e_i \to e_j) = \begin{cases} \frac{1}{\deg(\mathrm{out}(e_i))-1} & \text{if } \mathrm{out}(e_i) = \mathrm{in}(e_j) \text{ and } \mathrm{in}(e_i) \neq \mathrm{out}(e_j) \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, the nonbacktracking matrix of G can be defined directly, without first considering the nonbacktracking graph, in the following way.

Definition 12.1.2. The matrix $B := B(G)$ is the $2M \times 2M$ matrix with $(0,1)$–entries such that

$$B_{ij} = 1 \iff \mathrm{out}(e_i) = \mathrm{in}(e_j) \text{ and } \mathrm{in}(e_i) \neq \mathrm{out}(e_j).$$

The *nonbacktracking matrix* of G is $B^\top$, the transpose matrix of B.

Now, we fix a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ on $\mathcal{N}$ nodes and $\mathcal{M}$ edges. If $\mathcal{G}$ has an edge from a vertex v to a vertex w, we write $v \to w$ and denote such an edge by $(v \to w)$. Given a vertex $v \in \mathcal{V}$, we define its *outdegree* or simply its *degree* as

$$\deg_{\mathcal{G}} v := \deg v := |\{w \in \mathcal{V} \colon (v \to w) \in \mathcal{E}\}|.$$

We assume that $\mathcal{G}$ has minimum degree ≥ 1, and, analogously to the undirected case, we define the following operators.

We now recall the definitions from Section 4.7.

Definition 12.1.3. The *degree matrix* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ diagonal matrix $\mathcal{D} := \mathcal{D}(\mathcal{G}) := (\mathcal{D}_{vw})_{v,w \in \mathcal{V}}$ whose diagonal entries are

$$\mathcal{D}_{vv} := \deg v.$$

The *adjacency matrix* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ matrix $\mathcal{A} := \mathcal{A}(\mathcal{G}) := (\mathcal{A}_{vw})_{v,w \in \mathcal{V}}$ defined by

$$\mathcal{A}_{vw} := \begin{cases} 1 & \text{if } v \to w \\ 0 & \text{otherwise.} \end{cases} \tag{12.1.1}$$

The *normalized Laplacian* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ matrix

$$\mathcal{L}(\mathcal{G}) := \mathrm{Id} - \mathcal{D}^{-1}\mathcal{A}. \tag{12.1.2}$$

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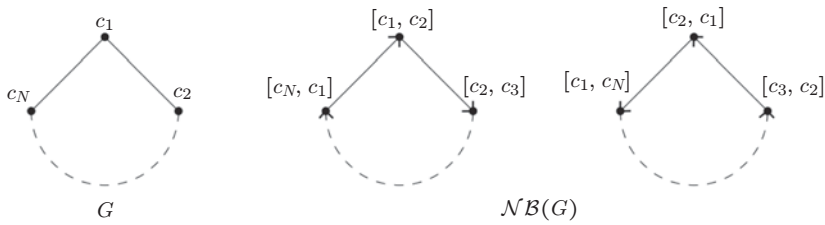


Figure 12.1 The cycle graph G and its nonbacktracking graph $\mathcal{NB}(G)$.

Remark 12.1.1. Similarly to the undirected case, the normalized Laplacian $\mathcal{L}$ of the directed graph $\mathcal{G}$ can be equivalently seen as an operator such that, given $f\colon \mathcal{V} \to \mathbb{C}$ and $\omega \in \mathcal{V}$,

$$\mathcal{L}f(\omega) = f(\omega) - \frac{1}{\deg \omega}\left(\sum_{\omega \to \tau} f(\tau)\right).$$

We can now define the nonbacktracking graph and the nonbacktracking Laplacian of G.

Definition 12.1.4. The *nonbacktracking graph* of G is the directed graph $\mathcal{NB}(G)$ on vertices $e_1, \ldots, e_{2M}$, that has B as its adjacency matrix.

The *nonbacktracking Laplacian* of G, denoted by $\mathcal{L} := \mathcal{L}(G)$, is the normalized Laplacian $\mathcal{L}(\mathcal{NB}(G))$ of $\mathcal{NB}(G)$.

Example 12.1.1. If G is the cycle graph on N nodes, then $\mathcal{NB}(G)$ is given by two disconnected directed cycles on N nodes (Figure 12.1).

Example 12.1.2. In this example, we consider a tripod (Figure 12.2). The tripod has pending vertices, that is, vertices of degree 1, and hence violates our general assumption that all vertices have degree at least 2, and therefore, the associated nonbacktracking graph is not strongly connected. The vertices corresponding to the oriented edges going out of the central node in the tripod have only incoming arrows but no outgoing ones, and conversely, the vertices corresponding to oriented edges into the central node have only outgoing arrows.

Example 12.1.3. We next consider a graph that has more than one cycle (Figure 12.3). If we want to traverse the oriented edge from v to w in the backward direction, we can simply go around the other cycle, return to w, and then go back to v. This is a nonbacktracking path.

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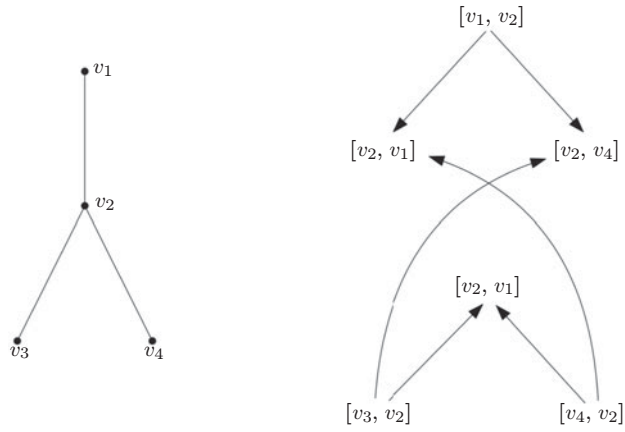


Figure 12.2 The tripod and its nonbacktracking graph.

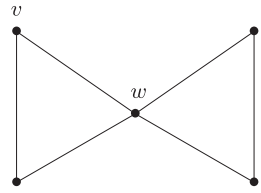


Figure 12.3 A graph that has more than one cycle.

In order to employ a systematic notation, we shall denote the nonbacktracking graph of $G = (V, E)$ by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. Clearly, if G has N nodes and M edges, then $\mathcal{G}$ has $2M$ nodes. Moreover, for each oriented edge e_i,

$$\deg_{\mathcal{G}} e_i = \deg_G(\text{out}(e_i)) - 1. \tag{12.1.3}$$

Hence, the assumption that G has minimum degree ≥ 2 implies that $\mathcal{G}$ has minimum degree ≥ 1. In particular, this assumption makes the nonbacktracking Laplacian well-defined.

Remark 12.1.2. The off-diagonal entries of the nonbacktracking Laplacian of G are given by

$$\mathcal{L}_{ij} = -\frac{B_{ij}}{\deg_{\mathcal{G}}(e_i)} = -\frac{B_{ij}}{\deg_G(\text{out}(e_i)) - 1} = -\mathbb{P}(e_i \to e_j),$$

for $i \neq j$. Therefore, the nonbacktracking Laplacian encodes the probabilities of nonbacktracking random walks on G.

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Remark 12.1.3. The *line-digraph* constructed by Harary and Norman [126] is given by the nonbacktracking graph with the addition of all directed edges of the form $[v,w] \to [w,v]$.

12.2 The Nonbacktracking Graph

We now investigate some properties of nonbacktracking graphs. We fix again a simple graph $G = (V,E)$ on N nodes and M edges that has minimum degree ≥ 2, and we let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be its nonbacktracking graph. According to our construction, $\mathcal{G}$ has $2M$ nodes. Another straightforward property is that, by (12.1.3), G is $(k+1)$–regular if and only if $\mathcal{G}$ is k–regular. Similarly, G is bipartite if and only if $\mathcal{G}$ is bipartite, since G has odd-length cycles if and only if $\mathcal{G}$ has odd-length cycles. Moreover, as shown in [66] and [220], every simple graph can be uniquely reconstructed from its nonbacktracking graph.

Proposition 12.2.1 gives the number of (directed) edges of $\mathcal{G}$.

Proposition 12.2.1. *Let $G = (V,E)$ be a simple graph on N nodes and M edges, with minimum degree ≥ 2, and let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be its nonbacktracking graph. Then, $\mathcal{G}$ has $\sum_{v\in V}(\deg_G v)^2 - 2M$ edges.*

Proof By definitions of vertex degrees for G and $\mathcal{G}$,

$$|\mathcal{E}| = \sum_{e\in\mathcal{V}} \deg_{\mathcal{G}} e, \text{ while } M = \frac{\sum_{v\in V}\deg_G v}{2}.$$

Therefore,

$$|\mathcal{E}| = \sum_{e\in\mathcal{V}} \deg_{\mathcal{G}} e = \sum_{v\in V} \deg_G v \cdot (\deg_G v - 1) = \sum_{v\in V}(\deg_G v)^2 - 2M,$$

where the second equality holds because, for each $v \in V$, there are $\deg_G v$ oriented edges of the form $[w,v]$ and for each of these oriented edges, there are $\deg_G v - 1$ oriented edges of the form $[v,z]$ with $z \neq w$. □

Now, in Example 12.1.1, we saw that if G is a cycle graph, then its nonbacktracking graph is given by two disconnected cycles. Theorem 12.2.1 shows that this is the only case in which a connected simple graph has a disconnected nonbacktracking graph.

Theorem 12.2.1. *Let $G = (V,E)$ be a simple connected graph on N nodes and M edges, with minimum degree ≥ 2, and let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be its nonbacktracking graph. Then, the following are equivalent:*

1. G is not the cycle graph;

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2. *G has at least two cycles;*
3. *$\mathcal{G}$ is weakly connected; and*
4. *$\mathcal{G}$ is strongly connected.*

Proof Clearly, since the minimum degree in G is ≥ 2, the first two conditions are equivalent to each other. Moreover, 4 clearly implies 3, and, by Example 12.1.1, 3 implies 1. Hence, if we prove that 1 implies 4, we are done.

An essential observation in the proof to follow is that if v, v' are two neighboring vertices and if we go from v to v', we can return to v in a nonbacktracking manner by inserting a nonbacktracking path starting at and returning to v' but not passing through v. That path need not be a cycle itself but will of course contain some cycle. Figure 12.3 illustrates this.

In fact, we just need to show the following two properties because their combination will allow us to go from any oriented edge to any other oriented edge.

1. If (v_0, v_1) and (v'_0, v'_1) are edges, then for some orientations, say $[v_0, v_1]$ and $[v'_0, v'_1]$, we can go from one to the other in $\mathcal{G}$.
2. If $[v_0, v_1]$ is an oriented edge, we can go from it to the oppositely oriented edge $[v_1, v_0]$ in $\mathcal{G}$.

Now 1 directly follows from the connectedness of G. For 2, we start at $[v_0, v_1]$ and follow any nonbacktracking path. We never get stuck because we assume that G has no pending vertices and because all vertices have a degree of at least 2. G is finite, and so, such a path π_1 either returns onto itself before reaching v_0 again. In that case, by the earlier observation, we can use it to reverse direction without backtracking and return to v_1 and hence the oppositely oriented edge $[v_1, v_0]$. Or π_1 eventually returns to v_0. But since we assume that G is not a cycle, there must be some vertex (of degree at least 3) on that path π_1 where we can branch off into a different path π_2. That path again either returns onto itself before reaching v_0 again, in which case we can proceed as before, or it brings us back to π_1 at some other vertex of degree at least 3, which will allow us to reverse directions on π_1 and return to v_1 without going through v_0 first. Thus, in any case, we obtain 2. □

12.3 First Spectral Properties of the Nonbacktracking Laplacian

We first consider a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ on $\mathcal{N}$ nodes and minimum degree ≥ 1, which need not be the nonbacktracking graph associated with a simple graph. Since its normalized Laplacian $\mathcal{L}$ is an $\mathcal{N} \times \mathcal{N}$ matrix of trace $\mathcal{N}$, it

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has $\mathcal{N}$ eigenvalues (counted with algebraic multiplicity) that sum to $\mathcal{N}$. Moreover, by Proposition 3.2 in [23], the spectrum of $\mathcal{L}$ is contained in the complex disc $D(1,1)$, and therefore, the real eigenvalues are contained in $[0,2]$. Also, by Proposition 3.1 in [23], 0 is an eigenvalue for $\mathcal{L}$, and the constant functions $f : \mathcal{V} \to \mathbb{C}$ are the corresponding eigenfunctions. As a consequence, from the spectrum of $\mathcal{L}$, we can derive the number of connected components of $\mathcal{G}$. Notably, this does not hold for the adjacency matrix $\mathcal{A}$ of $\mathcal{G}$.

Another property of $\mathcal{L}$, which is the same as in the undirected case, is that if $\mathcal{G}$ is a directed bipartite graph, then the spectra of both $\mathcal{L}$ and $\mathcal{A}$ are symmetric. Therefore, in particular, 2 is an eigenvalue for $\mathcal{L}$ [156]. However, the other direction does not necessarily hold in the directed case: As shown in [156], there exist directed graphs that are not bipartite but have 2 as an eigenvalue of their normalized Laplacian.

Furthermore, it follows from (12.1.2) that the normalized Laplacian $\mathcal{L}$ and the adjacency matrix $\mathcal{A}$ of $\mathcal{G}$ satisfy:

(i) f is an eigenfunction for $\mathcal{A}$ with eigenvalue 0 if and only if f is an eigenfunction for $\mathcal{L}$ with eigenvalue 1;

(ii) If $\mathcal{G}$ is k–regular, then (λ, f) is an eigenpair for $\mathcal{A}$ if and only if $(1 - \frac{\lambda}{k}, f)$ is an eigenpair for $\mathcal{L}$.

All the earlier properties hold for any directed graph $\mathcal{G}$. From here on, we shall focus on the case of nonbacktracking graphs. In particular, we fix again a simple $G = (V,E)$ on N nodes and M edges that have minimum degree ≥ 2, and we let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be its nonbacktracking graph. Thus, $\mathcal{A}$ as defined in (12.1.1) is the adjacency matrix of $\mathcal{G}$ (equivalently, the transpose of the nonbacktracking matrix of G) and $\mathcal{L}$ from (12.1.2) is the normalized Laplacian of $\mathcal{G}$ (equivalently, the nonbacktracking Laplacian of G). Also, as in the previous chapters, we let A and L denote the adjacency matrix and the normalized Laplacian of G, respectively.

The first important consequence of the earlier observations for the case of nonbacktracking graphs is the following.

Remark 12.3.1. As observed in Section 12.2, G is regular if and only if $\mathcal{G}$ is regular. In this case, we know that the spectral properties of L and A are equivalent to each other, and by property (ii) above, also the spectral properties of $\mathcal{L}$ and $\mathcal{A}$ are equivalent to each other. But since it is known that, in the regular case, the eigenvalues of $\mathcal{A}$ can be recovered from those of A [172, 175], it follows that in this case also the spectral theory of $\mathcal{L}$ can be recovered from that of A or, equivalently, of L.

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Now, although the nonbacktracking Laplacian is not symmetric, as we shall see in Theorem 12.3.1, it satisfies the so-called *PT-symmetry* (where PT stands for parity-time), following the terminology in [36]. Before stating it, we define the $2M \times 2M$ matrix

$$P := \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}$$

It satisfies

$$P^2 = \mathrm{Id}, \qquad P^\top = P = P^{-1}, \tag{12.3.1}$$

and its eigenvalues are

$$\pm 1, \text{ each with multiplicity } M. \tag{12.3.2}$$

Moreover, for $\mathbf{x}, \mathbf{y} \in \mathbb{C}^{2M}$, we let $\langle \mathbf{x}, \mathbf{y} \rangle := \overline{\mathbf{x}}^\top \mathbf{y}$ be the usual complex inner product, and we define their *P-product* as

$$(\mathbf{x}, \mathbf{y})_P := \langle \mathbf{x}, P\mathbf{y} \rangle = \overline{\mathbf{x}}^\top P \mathbf{y}.$$

From (12.1.1), we observe

Lemma 12.3.1.

$$\left(\mathcal{A}^\top P\right)_{i,j} = \begin{cases} 1, & \text{if } \mathrm{in}(e_i) = \mathrm{in}(e_j),\ \mathrm{out}(e_i) \neq \mathrm{out}(e_j), \\ 0, & \text{otherwise}. \end{cases} \tag{12.3.3}$$

□

Next,

Theorem 12.3.1. *The nonbacktracking adjacency matrix $\mathcal{A}$ and the nonbacktracking Laplacian $\mathcal{L}$ of a graph satisfy*

1. $\mathcal{A}^\top = P\mathcal{A}P$ *and* $\mathcal{L}^\top = P\mathcal{L}P$;
2. $\mathcal{A}$ *and* $\mathcal{L}$ *are self-adjoint with respect to the P-product;*
3. *If* $\mathbf{x}$ *is an eigenvector of* $\mathcal{A}$ *or* $\mathcal{L}$ *for an eigenvalue* $\lambda \in \mathbb{C}$ *is not real, then*

$$\sum_{[v,w]} \overline{x_{[v,w]}} \cdot x_{[w,v]} = \sum_{i=1}^{M} \left(\overline{x_i} \cdot x_{i+M} + \overline{x_{i+M}} \cdot x_i \right) = 0.$$

Proof 1. Since for a nonbacktracking graph $\mathcal{G}$, we can pass from the oriented edge e_i to the oriented edge e_j precisely if we can pass from $-e_j$ to $-e_i$ (the oppositely oriented edges),

$$\mathcal{A}_{ij} = \mathcal{A}_{j+M,i+M}.$$

Similarly,

$$\mathcal{L}_{ij} = -\mathbb{P}(e_i \to e_j) = -\mathbb{P}(e_j^{-1} \to e_i^{-1}) = \mathcal{L}_{j+M,i+M}.$$

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for $i \neq j$, $i, j \leq M$. These relations imply

$$\mathcal{A}^\top = P\mathcal{A}P, \quad \mathcal{L}^\top = P\mathcal{L}P. \tag{12.3.4}$$

2. With (12.3.4) and $P^\top = P$, we compute

$$\begin{aligned}(\mathbf{x}, \mathcal{A}\mathbf{y})_P &= \langle \mathbf{x}, P\mathcal{A}\mathbf{y}\rangle = \langle P\mathbf{x}, \mathcal{A}\mathbf{y}\rangle = \langle \mathcal{A}^\top P\mathbf{x}, \mathbf{y}\rangle \\ &= \langle P\mathcal{A}P^2\mathbf{x}, \mathbf{y}\rangle = \langle P\mathcal{A}\mathbf{x}, \mathbf{y}\rangle = \langle \mathcal{A}\mathbf{x}, P\mathbf{y}\rangle = (\mathcal{A}\mathbf{x}, \mathbf{y})_P.\end{aligned}$$

and analogously

$$(\mathbf{x}, \mathcal{L}\mathbf{y})_P = (\mathcal{L}\mathbf{x}, \mathbf{y})_P.$$

Therefore, $\mathcal{A}$ and $\mathcal{L}$ are self-adjoint with respect to the P-product.

3. The second claim implies that, if $(\lambda, \mathbf{x})$ is an eigenpair for $\mathcal{L}$, then

$$\lambda(\mathbf{x}, \mathbf{x})_P = (\mathbf{x}, \lambda\mathbf{x})_P = (\mathbf{x}, \mathcal{L}\mathbf{x})_P = (\mathcal{L}\mathbf{x}, \mathbf{x})_P = (\lambda\mathbf{x}, \mathbf{x})_P = \overline{\lambda}(\mathbf{x}, \mathbf{x})_P$$

and, of course, the analogous result holds for $\mathcal{A}$.

Hence, if $\lambda \neq \overline{\lambda}$, that is, λ is not real, then $(\mathbf{x}, \mathbf{x})_P = 0$, that is, $\overline{\mathbf{x}}^\top P\mathbf{x} = 0$, which can be rewritten as

$$\sum_{[v,w]} \overline{x_{[v,w]}} \cdot x_{[w,v]} == \sum_{i=1}^{m} \left(\overline{x_i} \cdot x_{i+M} + \overline{x_{i+M}} \cdot x_i\right) = 0.$$

□

12.4 Spectral Gap from 1

In Chapter 4, we have considered the spectral gap from the value 1 for the spectrum of the normalized Laplacian of a simple graph. We have seen that there exist simple graphs that have 1 as an eigenvalue; therefore, the spectral gap from 1 can be 0, and we have also seen (in Theorem 4.1.2) that this gap cannot be larger than $1/2$. In this section, we shall see that, in the case of the nonbacktracking Laplacian, things change.

Again, let $G = (V, E)$ be a simple graph on N nodes and M edges with minimum degree ≥ 2, let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be its nonbacktracking graph, and let $\mathcal{A}$ and $\mathcal{L}$ be its nonbacktracking matrix and its nonbacktracking Laplacian, respectively. Given an operator $\mathcal{O}$, let also $\sigma(\mathcal{O})$ denote its spectrum, and let $\rho(\mathcal{O})$ denote its spectral radius, that is, the largest modulus of its eigenvalues.

It is known that, by the assumption that G has minimum degree ≥ 2, 0 is not in the spectrum of $\mathcal{A}$ [261]. This implies that 1 is not in the spectrum of $\mathcal{L}$ and, therefore, the spectral gap from 1 for $\mathcal{L}$,

$$\varepsilon := \min_{\lambda \in \sigma(\mathcal{L})} |1 - \lambda| = \min_{\mu \in \sigma(\mathcal{D}^{-1}\mathcal{A})} |\mu|, \tag{12.4.1}$$

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is nonzero. In Theorem, 12.4.1 we give a lower bound for ε, and we prove that the bound is sharp. We also refer to [220] for the study of a sharp upper bound. Before stating the theorem, we prove Lemma 12.4.1. It uses the matrix P defined in Section 12.3, which satisfies $P\mathcal{A}P = \mathcal{A}^*$ and $P\mathcal{L}P = \mathcal{L}^*$.

Lemma 12.4.1. *The spectrum of $\mathcal{A}P$ is given by $\{-1\} \cup \{\deg v - 1\}_{v\in V}$, where each positive eigenvalue d has multiplicity equal to the number of nodes v with $\deg v - 1 = d$, and the multiplicity of -1 equals $2M - N$.*

Proof Note that the spectrum of $\mathcal{A}P$ equals the spectrum of $P^\top\mathcal{A}^\top = P\mathcal{A}^\top$, which equals the spectrum of $\mathcal{A}^\top P$, since 0 is not an eigenvalue.

With (12.3.3), the eigenproblem $\mathcal{A}^\top Pf = \lambda f$ simplifies to the system of equations

$$(\lambda + 1)\, f(e) = \sum_{\mathrm{in}(e')=\mathrm{in}(e)} f(e'), \text{ for each } e \in \mathcal{V}. \tag{12.4.2}$$

First fix a node $v \in V$ with degree d and define the function $f_v \colon \mathcal{V} \to \mathbb{R}$ by

$$f_v(e) \coloneqq \begin{cases} d, & \text{if } \mathrm{in}(e) = v \\ 0, & \text{otherwise.} \end{cases}$$

Then, f_v satisfies Equation (12.4.2) with eigenvalue $\lambda = d - 1$, and the set $\{f_v\}_{v\in V}$ is linearly independent. In other words, $\lambda = \deg v - 1$ is an eigenvalue of $\mathcal{A}^\top P$, for each node v, and each such eigenvalue has multiplicity equal to the number of nodes v with the corresponding degree.

Now fix an oriented edge $[v, w]$ with $v, w \in V$ and suppose v has degree d. Define the function $g_{[v,w]} \colon \mathcal{V} \to \mathbb{R}$ by

$$g_{[v,w]}(e) \coloneqq \begin{cases} -1, & \text{if } \mathrm{in}(e) = v,\ \mathrm{out}(e) = w \\ \frac{1}{d-1}, & \text{if } \mathrm{in}(e) = v,\ \mathrm{out}(e) \neq w \\ 0, & \text{otherwise.} \end{cases}$$

Then, $g_{[v,w]}$ satisfies equations (12.4.2) for the eigenvalue $\lambda = -1$. Now fix $v \in V$ and let $w_1, \ldots, w_d$ be its neighbors. It is clear that the matrix

$$[g_{[v,w_1]} | \ldots | g_{[v,w_d]}]$$

has rank $d - 1$. Furthermore, for two different nodes v and v', the vectors $g_{[v,w]}$ and $g_{[v',w']}$ are linearly independent. We have shown that the set $\{g_{[v,w]}\}_{v\sim w\in E}$, which contains $2M$ elements, contains exactly $\sum_v (\deg v - 1) = 2M - N$ linearly independent eigenfunctions of $\lambda = -1$, and we are done. □

Corollary 12.4.1. *$\mathcal{A}$ has both $+1$ and -1 as eigenvalues.*

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Proof By (12.3.2), P has ± 1 as the only eigenvalues, both with multiplicity M. We also have $M \geq N$ because we assume that every vertex has degree ≥ 2. And, $M = N$ then only occurs for a cycle graph, for which we shall give the argument later. Thus, by Lemma 12.4.1, we may assume that the multiplicity of the eigenvalue -1 of $\mathcal{A}P$ is $> M$. But then, this eigenspace must contain eigenvectors of P for both eigenvalues $+1$ and -1, and since $\mathcal{A} = (\mathcal{A}P)P$, we then get both eigenvalues $+1$ and -1 for $\mathcal{A}$ as well.

In the case of the cycle graph, all vertices have degree 2, and so, by Lemma 12.4.1 again, $\mathcal{A}P$ has the two eigenvalues ± 1 with multiplicity $M = N$, and we can apply a similar argument. □

As a consequence of Lemma 12.4.1,

$$\min_{\lambda \in \sigma(\mathcal{A}P)} |\lambda|^2 = 1.$$

Theorem 12.4.1. *Let G be a simple graph with maximum vertex degree Δ. Then, the spectral gap* (12.4.1) *from* 1 *for the nonbacktracking Laplacian $\mathcal{L}$ of G satisfies*

$$\varepsilon \geq \frac{1}{\Delta - 1}.$$

This bound is sharp.

Proof Since $0 \notin \sigma(\mathcal{A})$, the matrix $\mathcal{A}$ is invertible. Therefore, we can write

$$\varepsilon^{-1} = \max_{\lambda \in \sigma(\mathcal{D}\mathcal{A}^{-1})} |\lambda| = \rho(\mathcal{D}\mathcal{A}^{-1}).$$

Further, the spectral norm $\|\cdot\|_2$

$$\rho\left(\mathcal{D}\mathcal{A}^{-1}\right) \leq \|\mathcal{D}\mathcal{A}^{-1}\| \leq \|\mathcal{D}\|\|\mathcal{A}^{-1}\|.$$

The nonbacktracking diagonal matrix $\mathcal{D}$ satisfies$\|\mathcal{D}\|_2 = \Delta - 1$. And $\|\mathcal{A}^{-1}\|_2^2$ equals the largest norm among the eigenvalues of $\left(\mathcal{A}^{-1}\right)^* \mathcal{A}^{-1}$. But, by (12.3.4), $\mathcal{A}^\top = P\mathcal{A}P$, and thus,

$$\|\mathcal{A}^{-1}\|_2^2 = \max_{\mu \in \sigma\left(P\mathcal{A}^{-1}P\mathcal{A}^{-1}\right)} |\mu| = \max_{\nu \in \sigma\left(P\mathcal{A}^{-1}\right)} |\nu|^2 = \frac{1}{\min_{\lambda \in \sigma(\mathcal{A}P)} |\lambda|^2} = 1,$$

since the smallest norm of the eigenvalues of $\mathcal{A}P$ is 1, as shown in Lemma 12.4.1. Therefore,

$$\varepsilon^{-1} = \rho\left(\mathcal{D}\mathcal{A}^{-1}\right) \leq \|\mathcal{D}\|_2\|\mathcal{A}^{-1}\|_2 = \Delta - 1.$$

Thus, the spectral gap ε is at least $(\Delta - 1)^{-1}$.

To prove that the lower bound is sharp, we use the fact that ± 1 are always eigenvalues of $\mathcal{A}$ by Corollary 12.4.1. It follows that, if G is Δ–regular, then $1 \pm \frac{1}{\Delta - 1}$ are eigenvalues of $\mathcal{L}$. Hence, in particular, $\varepsilon = \frac{1}{\Delta - 1}$ in this case. □

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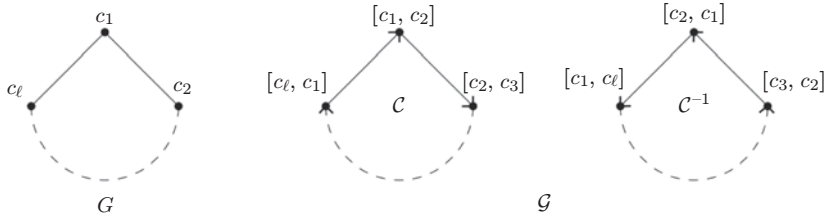


Figure 12.4 The setting of Section 12.5.

In the proof of Theorem 12.4.1, we have shown that, if G is Δ–regular, then $1 \pm \frac{1}{\Delta-1}$ are two real eigenvalues of $\mathcal{L}$. A natural question is whether regular graphs are the only graphs for which $\varepsilon = \frac{1}{\Delta-1}$, but the answer is no. In the next section, we show that, for instance, the presence of a Δ–regular cycle in the graph G produces the eigenvalues $1 \pm \frac{1}{\Delta-1}$ for $\mathcal{L}$.

12.5 Cycles

This section is dedicated to the signature that cycles can leave in the spectrum of the nonbacktracking Laplacian. As before, we consider a simple graph $G = (V, E)$ on N nodes and M edges that has minimum degree ≥ 2, and we let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be its nonbacktracking graph. We start with the following observation.

Remark 12.5.1. We say that a cycle is *chordless* if no two vertices of the cycle are connected by an edge that does not belong to the cycle. Given $c_1, \dots, c_\ell \in V$, then, as already observed in Example 12.1.1 and illustrated in Figure 12.4,

$$\{c_1, \dots, c_\ell\} \text{is a simple chordless cycle in } G \iff \mathcal{C} := \{[c_1, c_2], \dots, [c_\ell, c_1]\}$$
is a simple chordless cycle in $\mathcal{G}$
$$\iff \text{both } \mathcal{C} \text{ and } \mathcal{C}^{-1} := \{[c_1, c_\ell], \dots, [c_2, c_1]\}$$
are simple chordless cycles in $\mathcal{G}$.

Moreover, $\mathcal{C} \cap \mathcal{C}^{-1} = \emptyset$ and there are no edges between $\mathcal{C}$ and $\mathcal{C}^{-1}$ in $\mathcal{G}$.

From here on, we also fix $\mathcal{C}$ and $\mathcal{C}^{-1}$ as mentioned earlier. Lemma 12.5.1 concerns a structural property of $\mathcal{G}$ related to the vertices outside $\mathcal{C} \sqcup \mathcal{C}^{-1}$:

Lemma 12.5.1. *If $e \in \mathcal{V} \setminus \left(\mathcal{C} \sqcup \mathcal{C}^{-1}\right)$, then exactly one of the following holds:*

1. *There are no edges between e and $\mathcal{C} \sqcup \mathcal{C}^{-1}$ in $\mathcal{G}$;*
2. *There exists $i \in \{1, \dots, \ell\}$ such that the only edge between e and $\mathcal{C}$ is $(e \to [c_i, c_{i+1}])$, while the only edge between e and $\mathcal{C}^{-1}$ is $(e \to [c_i, c_{i-1}])$ (Figure 12.5); and*

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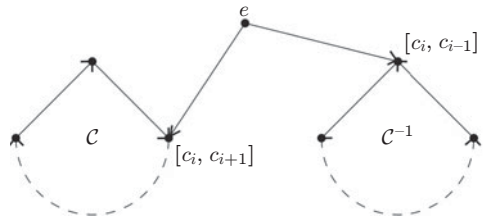


Figure 12.5 An illustration of Lemma 12.5.1.

3. *There exists* $i \in \{1,\dots,\ell\}$ *such that the only edge between* e *and* $\mathcal{C}$ *is* $([c_{i-1},c_i] \to e)$*, while the only edge between* e *and* $\mathcal{C}^{-1}$ *is* $([c_{i+1},c_i] \to e)$.

Proof This essentially follows from the fact that each directed edge has a unique beginning and end and obvious symmetry considerations. Here are the details:

Assume that there exists a directed edge going from e to $\mathcal{C} \sqcup \mathcal{C}^{-1}$ in $\mathcal{G}$ and assume, without loss of generality, that this directed edge goes to $\mathcal{C}$. Then, there exists $i \in \{1,\dots,\ell\}$ such that $(e \to [c_i,c_{i+1}]) \in \mathcal{E}$. This implies that $\mathrm{out}(e) = c_i$ and $\mathrm{in}(e) \neq c_{i-1},c_{i+1}$, since we are assuming that $e \notin \mathcal{C} \sqcup \mathcal{C}^{-1}$. Therefore, $(e \to [c_i,c_{i-1}]) \in \mathcal{E}$. Moreover, since $\mathrm{out}(e) = c_i$ and $\mathrm{in}(e) \neq c_{i-1},c_{i+1}$, it is clear that there cannot be other edges between e and $\mathcal{C} \sqcup \mathcal{C}^{-1}$, other than $(e \to [c_i,c_{i+1}])$ and $(e \to [c_i,c_{i-1}])$.

In the same way, one can show that if there exists a directed edge going from $\mathcal{C} \sqcup \mathcal{C}^{-1}$ to e in $\mathcal{G}$, then there exists $i \in \{1,\dots,\ell\}$ such that the only edge between e and $\mathcal{C}$ is $([c_{i-1},c_i] \to e)$, while the only edge between e and $\mathcal{C}^{-1}$ is $([c_{i+1},c_i] \to e)$. This proves the claim. □

Lemmas 12.5.2 and 12.3.1 will allow us to prove Theorem 12.5.1, which shows that the presence of a d–regular cycle in the graph G produces the eigenvalues $1 \pm \frac{1}{d-1}$ for $\mathcal{L}$, as anticipated in Section 12.4.

Lemma 12.5.2. *Let* $\mu \in \mathbb{R} \setminus \{0\}$ *and let* $f : \mathcal{V} \to \mathbb{R}$, $f \neq \mathbf{0}$ *be a function whose support is contained in* $\mathcal{C} \sqcup \mathcal{C}^{-1}$*. Then,* $(1 - \frac{1}{\mu}, f)$ *is an eigenpair for* $\mathcal{L}$ *if and only if the following conditions hold:*

1.
$$f([c_{i-1},c_i]) = \frac{\mu}{\deg c_i - 1} \cdot f([c_i,c_{i+1}]), \quad \forall i \in \{1,\dots,\ell\};$$

2.
$$f([c_{i+1},c_i]) = \frac{\mu}{\deg c_i - 1} \cdot f([c_i,c_{i-1}]), \ \forall i \in \{1,\dots,\ell\}; \text{ and}$$

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3.

$$f([c_i, c_{i+1}]) + f([c_i, c_{i-1}]) = 0, \quad \forall i \in \{1, \dots, \ell\} \colon \deg c_i > 2.$$

Proof $(1 - \frac{1}{\mu}, f)$ is an eigenpair for $\mathcal{L}$ if and only if

$$f([v, w]) = \frac{\mu}{\deg w - 1} \cdot \left(\sum_{[w,z],\, z \neq v} f([w, z]) \right), \quad \forall [v, w]. \tag{12.5.1}$$

Since, by assumption, the support of f is contained in $\mathcal{C} \sqcup \mathcal{C}^{-1}$, (12.5.1) applied to the vertices in $\mathcal{C} \sqcup \mathcal{C}^{-1}$ gives the first two claims.

Now, let $e = [v, w] \in \mathcal{V} \setminus \left(\mathcal{C} \sqcup \mathcal{C}^{-1} \right)$. If there are no directed edges from e to $\mathcal{C} \sqcup \mathcal{C}^{-1}$ in $\mathcal{G}$, then (12.5.1) is trivially satisfied. Otherwise, by Lemma 12.5.1, there exists $i \in \{1, \dots, \ell\}$ such that the only edge from e to $\mathcal{C}$ is $(e \to [c_i, c_{i+1}])$, while the only edge from e to $\mathcal{C}^{-1}$ is $(e \to [c_i, c_{i-1}])$. This happens if and only if $\mathrm{out}(e) = c_i$, and, in this case, (12.5.1) becomes

$$f([c_i, c_{i+1}]) + f([c_i, c_{i-1}]) = 0.$$

Since an element $e \in \mathcal{V} \setminus \left(\mathcal{C} \sqcup \mathcal{C}^{-1} \right)$ with $\mathrm{out}(e) = c_i$ exists if and only if $\deg c_i > 2$, this proves the last claim.

□

Corollary 12.5.1. *Let $\mu \in \mathbb{R}_+$ and let $f \colon \mathcal{V} \to \mathbb{R}$, $f \neq \mathbf{0}$ be a function whose support is contained in $\mathcal{C} \sqcup \mathcal{C}^{-1}$, where $\mathcal{C}$ has even length. If $(1 - \frac{1}{\mu}, f)$ is an eigenpair for $\mathcal{L}$, then also $1 + \frac{1}{\mu}$ is an eigenvalue for $\mathcal{L}$ and it has an eigenfunction whose support is contained in $\mathcal{C} \sqcup \mathcal{C}^{-1}$.*

Proof Let $g \colon \mathcal{V} \to \mathbb{R}$ be defined by $g(e) \coloneqq 0$ if $e \in \mathcal{V} \setminus \left(\mathcal{C} \sqcup \mathcal{C}^{-1} \right)$ and

$$g([c_i, v]) \coloneqq \begin{cases} f([c_i, v]), & \text{if } i \text{ is even} \\ -f([c_i, v]), & \text{if } i \text{ is odd,} \end{cases}$$

for $i = 1, \dots, \ell$. Then, g satisfies the conditions in Lemma 12.5.2 for $1 + \frac{1}{\mu}$. □

We can now identify conditions for cycles to generate eigenpairs. We first prove the following result on regular cycles:

Theorem 12.5.1. *Let $d > 1$. If there exists a simple chordless cycle in G whose vertices have constant degree d, then $1 - \frac{1}{d-1}$ is an eigenvalue for $\mathcal{L}$. If, additionally, such a cycle is even, then also $1 + \frac{1}{d-1}$ is an eigenvalue for $\mathcal{L}$.*

Moreover, the geometric multiplicity of $1 - \frac{1}{d-1}$ for $\mathcal{L}$ is larger than or equal to the number of d–regular simple chordless cycles in G, while the geometric multiplicity of $1 + \frac{1}{d-1}$ for $\mathcal{L}$ is larger than or equal to the number of d–regular even simple chordless cycles in G.

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Proof Given a cycle whose vertices have constant degree d, let $f\colon \mathcal{V} \to \mathbb{R}$ be defined by

$$f(e) \coloneqq \begin{cases} 1 & \text{if } e \in \mathcal{C} \\ -1 & \text{if } e \in \mathcal{C}^{-1} \\ 0 & \text{otherwise.} \end{cases}$$

Then, f satisfies the conditions in Lemma 12.5.2 for the eigenvalue $1 - \frac{1}{d-1}$, implying that $(1 - \frac{1}{d-1}, f)$ is an eigenpair for $\mathcal{L}$. This proves the first claim for $1 - \frac{1}{d-1}$, and the first claim for $1 + \frac{1}{d-1}$ then follows from Corollary 12.5.1.

The second claim follows from the fact that the preceding functions are linearly independent if they are defined for distinct cycles. □

The next result is proved in a similar way.

Theorem 12.5.2. *Let $d > 2$. If there exists a simple chordless cycle of length ℓ in G such that one vertex has degree d while all other vertices have degree 2, then $1 - \frac{1}{\sqrt[\ell]{d-1}}$ is an eigenvalue for $\mathcal{L}$. If, additionally, such a cycle is even, then also $1 + \frac{1}{\sqrt[\ell]{d-1}}$ is an eigenvalue for $\mathcal{L}$.*

Moreover, the geometric multiplicity of $1 - \frac{1}{\sqrt[\ell]{d-1}}$ for $\mathcal{L}$ is larger than or equal to the number of such cycles in G, while the geometric multiplicity of $1 + \frac{1}{\sqrt[\ell]{d-1}}$ for $\mathcal{L}$ is larger than or equal to the number of such even cycles in G.

Proof Fix a cycle $\{c_1, \dots, c_\ell\}$ in G and let

$$\mathcal{C} \coloneqq \{[c_1, c_2], \dots, [c_\ell, c_1]\}, \quad \mathcal{C}^{-1} \coloneqq \{[c_1, c_\ell], \dots, [c_2, c_1]\}$$

be the corresponding cycles in $\mathcal{G}$. Let $c_0 \coloneqq c_\ell$ and $c_{\ell+1} \coloneqq c_1$, and assume that $\deg c_1 = d > 2$, while $\deg c_i = 2$ for $i \in \{2, \dots, \ell\}$. The proof is similar to the one of Theorem 12.5.1. In this case, we can apply Lemma 12.5.2 for $\mu = \sqrt[\ell]{d-1}$ if we find a nonzero function $f\colon \mathcal{V} \to \mathbb{R}$ whose support is contained in $\mathcal{C} \sqcup \mathcal{C}^{-1}$ and such that the following conditions hold:

1.
$$f([c_\ell, c_1]) = \frac{\sqrt[\ell]{d-1}}{d-1} \cdot f([c_1, c_2]);$$

2.
$$f([c_{i-1}, c_i]) = \sqrt[\ell]{d-1} \cdot f([c_i, c_{i+1}]), \quad \forall i \in \{2, \dots, \ell\};$$

3.
$$f([c_2, c_1]) = \frac{\sqrt[\ell]{d-1}}{d-1} \cdot f([c_1, c_\ell]);$$

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4.
$$f([c_{i+1},c_i]) = \sqrt[\ell]{d-1}\cdot f([c_i,c_{i-1}]), \quad \forall i \in \{2,\dots,\ell\};$$

5.
$$f([c_1,c_2]) + f([c_1,c_\ell]) = 0.$$

By letting
$$\begin{aligned}
f([c_1,c_2]) &\coloneqq -f([c_1,c_\ell]) \coloneqq 1,\\
f([c_\ell,c_1]) &\coloneqq -f([c_2,c_1]) \coloneqq \frac{\sqrt[\ell]{d-1}}{d-1},\\
f([c_{\ell-1},c_\ell]) &\coloneqq \sqrt[\ell]{d-1}\cdot f([c_\ell,c_1]),\\
&\vdots\\
f([c_2,c_3]) &\coloneqq \sqrt[\ell]{d-1}\cdot f([c_3,c_4]),\\
f([c_3,c_2]) &\coloneqq \sqrt[\ell]{d-1}\cdot f([c_2,c_1]),\\
&\vdots\\
f([c_\ell,c_{\ell-1}]) &\coloneqq \sqrt[\ell]{d-1}\cdot f([c_{\ell-1},c_{\ell-2}]),
\end{aligned}$$

then clearly conditions 1, 2, and 5 above are satisfied, as well as condition 2 and for $i \in \{3,\dots,\ell\}$ and condition 4 for $i \in \{2,\dots,\ell-1\}$. Moreover, since
$$\begin{aligned}
\sqrt[\ell]{d-1}\cdot f([c_2,c_3]) &= \sqrt[\ell]{d-1}\cdot\sqrt[\ell]{d-1}\cdot f([c_3,c_4])\\
&= (\sqrt[\ell]{d-1})^{\ell-1}\cdot f([c_\ell,c_1])\\
&= (\sqrt[\ell]{d-1})^{\ell-1}\cdot\frac{\sqrt[\ell]{d-1}}{d-1}\\
&= 1 = f([c_1,c_2]),
\end{aligned}$$

the second condition is satisfied also for $i = 2$. Similarly, since
$$\sqrt[\ell]{d-1}\cdot f([c_\ell,c_{\ell-1}]) = (\sqrt[\ell]{d-1})^{\ell-1}\cdot f([c_2,c_1]) = -1 = f([c_1,c_\ell]),$$

the fourth condition is satisfied also for $i = \ell$. By using the same method as in the proof of Theorem 12.5.1, this proves the claim. □

The previous results show that certain chordless cycles $\mathcal{C}$ in $\mathcal{G}$ produce eigenvalues of the form $1 - \frac{1}{\mu}$ for $\mathcal{L}$, where μ is a positive real number that depends on the cycle structure. The corresponding eigenfunctions are supported in $\mathcal{C} \sqcup \mathcal{C}^{-1}$. But this does not generalize to all cycles. In fact, Theorem 12.5.3 completely characterizes those cycles for which it is possible.

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Theorem 12.5.3. *Assume that G is not a cycle graph. Let $\{c_1,\dots,c_\ell\}$ be a simple chordless cycle in G and let*

$$\mathcal{C} \coloneqq \{[c_1,c_2],\dots,[c_\ell,c_1]\}, \quad \mathcal{C}^{-1} \coloneqq \{[c_1,c_\ell],\dots,[c_2,c_1]\}$$

be the corresponding cycles in $\mathcal{G}$. Then, $\mathcal{L}$ admits an eigenpair of the form $(1-\frac{1}{\mu},f)$, where $\mu\in\mathbb{R}_+$ and $f\colon \mathcal{V}\to\mathbb{R}$ is a nonzero function with support in $\mathcal{C}\sqcup\mathcal{C}^{-1}$, if and only if

$$\mu = \sqrt[\ell]{(\deg c_1-1)\cdot(\deg c_2-1)\cdots(\deg c_\ell-1)}$$

and, after cyclically or anticyclically relabeling the vertices of the cycle, $\deg c_1>2$ and, for all $i\in\{2,\dots,\ell\}$ such that $\deg c_i>2$,

$$\begin{aligned}&\frac{\mu}{\deg c_{i+1}-1}\cdot\frac{\mu}{\deg c_{i+2}-1}\cdots\frac{\mu}{\deg c_\ell-1}\cdot\frac{\mu}{\deg c_1-1}\\ &=\frac{\mu}{\deg c_{i-1}-1}\cdot\frac{\mu}{\deg c_{i-2}-1}\cdots\frac{\mu}{\deg c_2-1}\cdot\frac{\mu}{\deg c_1-1}.\end{aligned}\tag{12.5.2}$$

Remark 12.5.2. In (12.5.2), there is a factor $\frac{\mu}{\deg c_1-1}$ on both sides. It cancels out, but writing it down helps understand the condition for $i=2$.

Proof of Theorem 12.5.3 Since G is not a cycle graph, then after relabeling the vertices of the cycle, we can assume that $\deg c_1>2$. In this case, $(1-\frac{1}{\mu},f)$ is an eigenpair for $\mathcal{L}$ if and only if they satisfy the conditions of Lemma 12.5.2. In particular, $f([c_1,c_2])\neq 0$, and we can assume that

$$f([c_1,c_2]) = 1.$$

The third condition of Lemma 12.5.2 applied to $i=1$ then gives

$$f([c_1,c_\ell]) = -1,$$

while the first condition applied to $i\neq 2$ gives

$$\begin{aligned}f([c_\ell,c_1]) &= \frac{\mu}{\deg c_1-1}\cdot f([c_1,c_2]) = \frac{\mu}{\deg c_1-1},\\ f([c_{\ell-1},c_\ell]) &= \frac{\mu}{\deg c_\ell-1}\cdot f([c_\ell,c_1]) = \frac{\mu}{\deg c_\ell-1}\cdot\frac{\mu}{\deg c_1-1},\\ &\vdots\\ f([c_2,c_3]) &= \frac{\mu}{\deg c_3-1}\cdot f([c_3,c_4]) = \frac{\mu}{\deg c_3-1}\cdots\frac{\mu}{\deg c_\ell-1}\cdot\frac{\mu}{\deg c_1-1},\end{aligned}$$

and the second condition of Lemma 12.5.2 applied to $i\neq\ell$ gives

$$f([c_2,c_1]) = \frac{\mu}{\deg c_1-1}\cdot f([c_1,c_\ell]) = -\frac{\mu}{\deg c_1-1},$$

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$$f([c_3,c_2]) = \frac{\mu}{\deg c_2 - 1} \cdot f([c_2,c_1]) = -\frac{\mu}{\deg c_2 - 1} \cdot \frac{\mu}{\deg c_1 - 1},$$

$$\vdots$$

$$\begin{aligned} f([c_\ell,c_{\ell-1}]) &= \frac{\mu}{\deg c_{\ell-1} - 1} \cdot f([c_{\ell-1},c_{\ell-2}]) \\ &= -\frac{\mu}{\deg c_{\ell-1} - 1} \cdot \frac{\mu}{\deg c_{\ell-2} - 1} \cdots \frac{\mu}{\deg c_1 - 1}. \end{aligned}$$

In particular, the earlier conditions give a complete description of f, given μ. We now check the other conditions of Lemma 12.5.2. We observe that:

1. The first condition of Lemma 12.5.2 is satisfied for all $i \in \{1,\dots,\ell\}$ if and only if

$$\begin{aligned} 1 = f([c_1,c_2]) &= \frac{\mu}{\deg c_2 - 1} \cdot f([c_2,c_3]) \\ &= \frac{\mu}{\deg c_2 - 1} \cdot \frac{\mu}{\deg c_3 - 1} \cdots \frac{\mu}{\deg c_\ell - 1} \cdot \frac{\mu}{\deg c_1 - 1}, \end{aligned}$$

that is, if and only if

$$\mu = \sqrt[\ell]{(\deg c_1 - 1) \cdot (\deg c_2 - 1) \cdots (\deg c_\ell - 1)};$$

2. The second condition of Lemma 12.5.2 is satisfied for all $i \in \{1,\dots,\ell\}$ if and only if

$$\begin{aligned} -1 = f([c_1,c_\ell]) &= \frac{\mu}{\deg c_\ell - 1} \cdot f([c_\ell,c_{\ell-1}]) \\ &= -\frac{\mu}{\deg c_\ell - 1} \cdot \frac{\mu}{\deg c_{\ell-1} - 1} \cdot \frac{\mu}{\deg c_{\ell-2} - 1} \cdots \frac{\mu}{\deg c_1 - 1}, \end{aligned}$$

that is, as before, if and only if

$$\mu = \sqrt[\ell]{(\deg c_1 - 1) \cdot (\deg c_2 - 1) \cdots (\deg c_\ell - 1)};$$

3. The third condition of Lemma 12.5.2 is satisfied if and only if, for all $i \in \{2,\dots,\ell\}$ such that $\deg c_i > 2$,

$$f([c_i,c_{i+1}]) = -f([c_i,c_{i-1}]), \tag{12.5.3}$$

where

$$f([c_i,c_{i+1}]) = \frac{\mu}{\deg c_{i+1} - 1} \cdot \frac{\mu}{\deg c_{i+2} - 1} \cdots \frac{\mu}{\deg c_\ell - 1} \cdot \frac{\mu}{\deg c_1 - 1}$$

and

$$-f([c_i,c_{i-1}]) = \frac{\mu}{\deg c_{i-1} - 1} \cdot \frac{\mu}{\deg c_{i-2} - 1} \cdots \frac{\mu}{\deg c_1 - 1},$$

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therefore (12.5.3) can be rewritten as

$$\frac{\mu}{\deg c_{i+1}-1}\cdot\frac{\mu}{\deg c_{i+2}-1}\cdots\frac{\mu}{\deg c_{\ell}-1}$$
$$=\frac{\mu}{\deg c_{i-1}-1}\frac{\mu}{\deg c_{i-2}-1}\cdots\frac{\mu}{\deg c_2-1}.$$

Putting everything together, we have that $1-\frac{1}{\mu}$ is an eigenvalue with an eigenfunction whose support is contained in $\mathcal{C}\sqcup\mathcal{C}^{-1}$ if and only if

$$\mu=\sqrt[\ell]{(\deg c_1-1)\cdot(\deg c_2-1)\cdots(\deg c_{\ell}-1)}$$

and (12.5.2) is satisfied for all $i\in\{2,\dots,\ell\}$ such that $\deg c_i>2$. □

12.6 Isospectrality

Recall that two graphs are said to be *isospectral* with respect to a given operator if they are nonisomorphic but have the same spectrum with respect to that operator. Hence, the smaller the number of isospectral graphs, the better the operator is at distinguishing nonisomorphic graphs. We recall that in Corollary 4.1.11, we have already seen some isospectral graphs, complete bipartite graphs with the same number of vertices, and for systematic constructions of isospectral graphs, we refer to [112, 258].

While we do not intend to present a systematic account of isospectral graphs in this book, we conclude this chapter by showing two isospectrality tables, which suggest that the nonbacktracking Laplacian has nicer isospectrality properties than the adjacency matrix, the normalized Laplacian, and the nonbacktracking matrix of a graph. We refer to [156] for the computational details.

In Tables 12.1 and 12.2, we show the number of simple graphs with minimum degree ≥ 2 not determined by their spectrum with respect to the

Table 12.1 *Graphs with minimum degree* ≥ 2 *not determined by their spectrum, by number of nodes* N.

N	#graphs	A	L	$\mathcal{A}$	$\mathcal{L}$
≤6	76	0	2	0	0
7	510	26	4	0	0
8	7 459	744	11	2	0
9	197 867	32 713	243	6	0
10	9 808 968	1 976 884	16 114	10 130	156
total	10 014 880	2 010 367	16 374	10 138	156

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Table 12.2 *Graphs with minimum degree* ≥ 2 *and* $4 \leq N \leq 10$ *not determined by their spectrum, by number of edges* M.

M	#graphs	$\mathcal{A}$	$\mathcal{L}$
0	0	0	0
1	0	0	0
2	0	0	0
3	0	0	0
4	1	0	0
5	2	0	0
6	6	0	0
7	10	0	0
8	25	0	0
9	68	0	0
10	182	0	0
11	532	0	0
12	1 679	0	0
13	5 218	4	0
14	15 437	14	0
15	41 126	26	0
16	96 274	62	0
17	197 433	162	0
18	355 986	364	4
19	567 827	634	8
20	807 284	983	16
21	1 029 639	1 329	24
22	1 184 688	1 492	26
23	1 235 599	1 490	26
24	1 172 658	1 333	24
25	1 015 663	989	16
26	804 863	628	8
27	584 762	368	4
28	390 136	166	0
29	239 514	60	0
30	135 636	26	0
31	71 025	8	0
32	34 559	0	0
33	15 734	0	0
34	6 745	0	0
35	2 764	0	0
36	1 101	0	0
≥ 37	704	0	0
total	10 014 880	10 138	156

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adjacency matrix A, to the normalized Laplacian L, to the nonbacktracking matrix $\mathcal{A}$ and to the nonbacktracking Laplacian $\mathcal{L}$. In Table 12.1, such graphs are partitioned by number of nodes N. In Table 12.2, graphs are partitioned by number of edges M. Interestingly, from Table 12.2, we can observe that the number of isospectral graphs with respect to $\mathcal{L}$ as a function of the number of edges M is in progression:

$$4, 8, 16, 24, 26, 26, 14, 16, 8, 4,$$

and in [156], it is conjectured that this is part of a larger pattern.

In Figures 12.6 and 12.7, we also illustrate the two smallest pairs of isospectral graphs with respect to the nonbacktracking Laplacian.

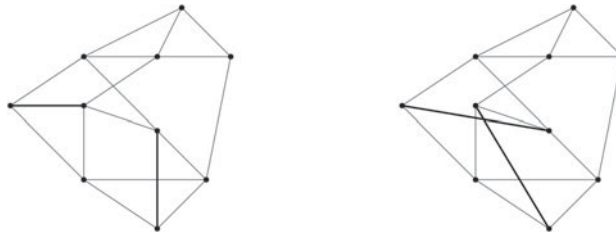


Figure 12.6 The first of the two smallest pairs of isospectral graphs with respect to $\mathcal{L}$.

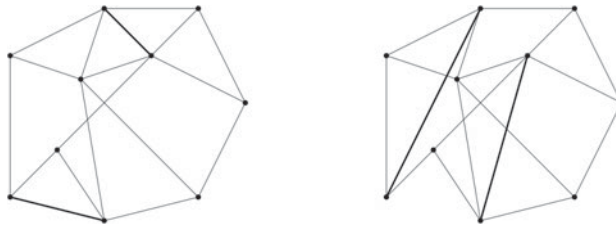


Figure 12.7 The second of the two smallest pairs of isospectral graphs with respect to $\mathcal{L}$.

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