PART 1

Dynamics on General Networks

1

Characterization of Networks: the Laplacian Matrix and its Functions

1.1. Introduction

The study of networks, their characteristics and dynamical processes taking place on these structures have had a significant impact in different fields of science and engineering, leading to important applications in the context of physics, biology and social and computer systems among many others. In this chapter, we present an introduction to several definitions in the context of the study of undirected connected networks that are used and discussed in various parts of this book. We start with an introduction to graph theory and concepts related to the connectivity of networks, in particular, the concept of distance in networks and the average of this quantity that gives a global characterization of the network connectivity. Different types of networks and their characteristics are described as well as three common algorithms to generate random networks.

In the second part of this chapter, the Laplacian matrix $\mathbf{L}$ of a network is discussed along with general properties of the eigenvalues and the respective eigenvectors of this matrix. The Laplacian matrix of a network has been explored in connection with dynamical processes on networks, in particular, diffusive transport and synchronization. Then we introduce a generalization of the notion of the "Laplacian matrix" and study a class of matrix functions $g(\mathbf{L})$ of the Laplacian matrix that maintains its structure and general "good" properties. We demonstrate that this generalization allows describing a rich variety of new dynamic processes that cannot be captured by the Laplacian matrix. In the framework of this generalization, we introduce the concept of the fractional Laplacian matrix, which is explored in detail in Chapter 2, and we work in terms of general Laplacian matrix functions in Chapter 4. In this way, we will define several types of random walk strategies with long-range displacements on networks.

1.2. Graph theory and networks

1.2.1. *Basic graph theory*

In order to study dynamical processes taking place on networks, it is necessary to work within a mathematical formalism called graph theory. In the past decades, graph theory and its applications in the context of networks have been an active field of research in science [NEW 10]. In general, a graph $\mathcal{G}$ is defined by a set of elements $\mathcal{V}$ of N nodes or vertices and a set of links or edges $\mathcal{E}$ composed of pairs of nodes [DIE 05]. In general, a graph can represent multiple lines between two nodes and loops connecting a node with itself. In Figure 1.1, we depict a graph illustrating these types of links between nodes.

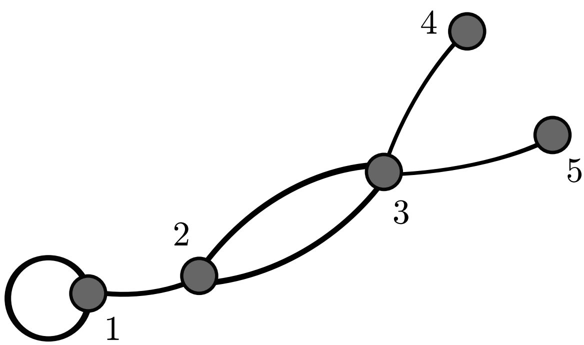

Figure 1.1. *A graph with multiple edges. The set of nodes is* $\mathcal{V} = \{1, 2, 3, 4, 5\}$ *and the set of edges is given by* $\mathcal{E} = \{\{1, 1\}, \{1, 2\}, \{2, 3\}, \{2, 3\}, \{3, 4\}, \{3, 5\}\}$

In addition to the sets $\mathcal{V}$ and $\mathcal{E}$, it is possible to incorporate additional information to a graph by assigning values to nodes and edges; in this case, we have a *weighted graph*. Also, when we consider the order of the pairs in the set of edges $\mathcal{E}$, the resulting structure is called a *directed graph*. A common graphical way to represent graphs is assigning a point for each node and connecting the nodes with lines according to the information in $\mathcal{E}$. For directed graphs, the direction of the line is represented by an arrow. The concept of graph constitutes an important tool to describe different types of complex systems since with these structures we can assign nodes to the parts of the system and represent the interactions between these parts through the use of edges.

In particular, an undirected graph without multiple edges and without loops is called a *simple graph*. Simple graphs with $i = 1, 2, \ldots, N$ nodes are represented in terms of an $N \times N$ adjacency matrix $\mathbf{A}$ with elements $A_{ij} = A_{ji} = 1$ if there exists an edge connecting the respective nodes, i.e. $\{i, j\} \in \mathcal{E}$, and $A_{ij} = 0$ when the respective nodes are not connected by an edge. In this structure, the diagonal elements satisfy $A_{ii} = 0$ as a direct consequence of the absence of loops in the whole structure. In simple graphs is defined the *degree* k_i of the node i as $k_i = \sum_{l=1}^{N} A_{il}$, and this value gives the number of connections with other nodes that i has; in addition, the set of nodes with direct links to i defines the *neighborhood* (or nearest-neighbors) of the node i and where when we mention "neighbor nodes" i, j, we mean connected nodes with $A_{ij} = 1$.

In the following, we present some definitions that allow us to describe how the nodes in a graph are connected [GRO 03]:

– A *path* in the graph $\mathcal{G}$ defined by the set of nodes $\mathcal{V}$ and edges $\mathcal{E}$ is a sequence of nodes and edges

$$\mathcal{W} = (v_0, e_1, v_1, \ldots, e_n, v_n),$$

where $\{v_i\}_{i=0}^{n} \subseteq \mathcal{V}$, $\{e_i\}_{i=1}^{n} \subseteq \mathcal{E}$. For $j = 1, \ldots, n$, the nodes v_{j-1} and v_j are the elements of the edge e_j. In simple graphs, a path is represented by a sequence of nodes $\mathcal{W} = (v_0, v_1, \ldots, v_n)$, with the additional condition that v_{j-1} and v_j are connected by an edge.

– A *cycle* in a graph is a path for which only the initial and final nodes coincide.

– The *distance* d_{ij} between nodes i, j in a graph is the number of edges of the shortest path connecting the nodes i, j.

– A graph is called *connected* if for each pair of nodes there exists at least one path connecting them.

– The *diameter* of a connected graph is the maximum distance between the nodes in the graph.

– The *average distance* between pairs of nodes in a simple connected graph is given by

$$\langle d \rangle \equiv \frac{1}{N(N-1)} \sum_{i=1}^{N} \sum_{j=1}^{N} d_{ij}.$$

In addition, it is worth noting that in several cases the shortest path connecting two nodes in a network is not unique.

Once these basic concepts are introduced to characterize the connectivity of a graph, we present the definition of some particular simple graphs that can be defined by using these terms. The following structures are used in different parts of the text:

– *Complete graph*: in this case, all the pairs of nodes are connected with an edge, and this is a fully connected structure. In terms of the adjacency matrix $\mathbf{A}$, the respective elements for a complete graph with N nodes are $A_{ij} = 1 - \delta_{ij}$ for $i, j = 1, 2, \ldots, N$, where δ_{ij} denotes the Kronecker delta.

– *Tree*: a tree is a connected graph without cycles.

– *Ring*: this is a graph defined by a cycle for which any node has only two neighbors.

– *Regular graph*: in a regular graph, each node has the same degree k. For example, a complete graph with N nodes is a regular graph with degrees $k = N - 1$. On the other hand, a ring is a regular graph with degree $k = 2$.

With these definitions, we have introduced some general concepts and terms of graph theory that will be useful in different parts of this book. In the next section, we apply this theory in connection with the study of networks.

1.2.2. *Networks*

In the following, we use the term *network* to denote simple connected graphs; in addition, variations of this term are common. For example, in directed networks we include information about the direction of the edges; on the other hand, the term weighted network refers to networks with additional information characterizing the nodes and strength of connections. In the last decade, the study of networks and its applications has started a revolution in the understanding of complex systems. The capacity of networks to describe a system in terms of its parts and interactions is of utmost importance and applications of this theory appear in the study of systems at different scales, from the microscopic world in the context of quantum transport, the structure of DNA and polymers, to macroscopic scales in the study of epidemic spreading, the structure of communication systems, social networks and the Internet, among a vast number of applications [NEW 10]. In terms of the connectivity, there are two special types of networks with $N \gg 1$ nodes: small-world networks, for which the average distance between pairs of nodes $\langle d \rangle \equiv \frac{1}{N(N-1)} \sum_{i,j} d_{ij}$ for N large scales as $\langle d \rangle \propto \log(N)$ and large-world networks with $\langle d \rangle$ that asymptotically scales as a power of the number of nodes N.

1.2.2.1. *Large-world networks*

In large-world networks, the average distance between nodes behaves asymptotically as a power of the number of nodes in the network; thus, distances between nodes are comparable to the size of the network and there are no nodes with connections that shorten distances in the whole structure limiting the network connectivity. Among the large-world networks are some trees, rings, square and triangular lattices, and well-known regular networks common in solid-state physics models. Another common group of large-world network is constituted by geometric random graphs that are obtained from randomly placing points in a plane and assigning as neighboring nodes the points that are in a circular region with a radius smaller than a fixed value R around each node [DAL 02]. For a particular interval of R, structures are obtained with the large-world property. On the other hand, in the context of search in networks, regular networks have been used with a fraction of lines removed; the resulting network is an irregular network with the large-world property. In Figure 1.2, we represent some of the large-world networks mentioned before; in Figure 1.2(a), we have a regular square lattice with degree $k = 4$, and in Figures 1.2(b) and (c), we have a tree and a random geometric graph.

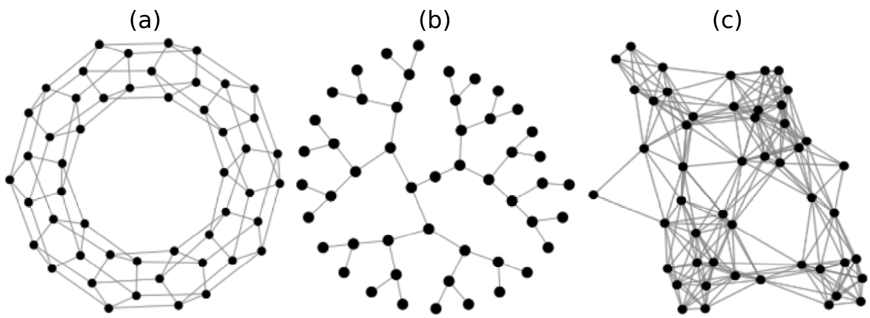

Figure 1.2. *Large-world networks with $N = 50$ nodes. (a) Regular square lattice with $k = 4$. (b) Tree. (c) Random geometric graph*

Other large-world networks are found in the study of fractal networks that arise by implementing various algorithms that can be deterministic or random. In the context of real networks, we find large-world networks in the analysis of transport networks like streets, subway stations, electric towers networks [NEW 10], pixels in digital images [GRA 06a], fractal networks in the modeling of glasses, proteins, among others.

1.2.2.2. *Small-world networks*

In small-world networks, the average distance between nodes is very small in comparison to the size N of the network. This property is common in several real networks and there are three typical models for creating random networks that capture this feature. These models are the random networks introduced by Erdös–Rényi (1959), Watts–Strogatz (1998) and Barabási–Albert (1999).

In the Erdös–Rényi model, we start with N nodes. The creation of lines between each pair of nodes depends on a fixed probability p to decide whether each pair of nodes is connected or not; these cases appear with probability p and $1-p$, respectively [ERD 59]. A random graph generated by this model for given values of N and p is denoted by $\mathcal{G}_{N,p}$. As an example, in Figure 1.3 we represent a random network with

$N = 1,000$ nodes generated by using this procedure with a probability $p = 0.0069$, and the resulting structure is a connected network.

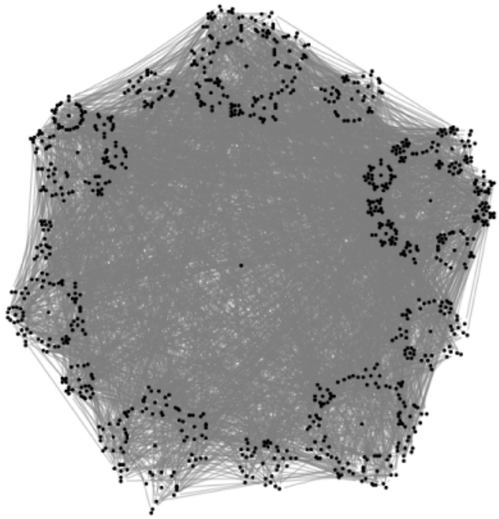

Figure 1.3. *Erdös–Rényi network with $N = 1,000$ nodes. We choose the percolation limit $p = \log(N)/N = 0.0069$ for the probability to establish links between pairs of nodes*

For an Erdös–Rényi network, the average value of the number of lines in $\mathcal{G}_{N,p}$ is $pN(N-1)/2$ and the average degree is $\langle k \rangle = p(N-1)$. On the other hand, the probability $P(k)$ to obtain a node with degree k is given by [BOL 01, BAR 08b]:

$$P(k) = \binom{N-1}{k} p^k (1-p)^{N-1-k} \approx \frac{\langle k \rangle^k \exp(-\langle k \rangle)}{k!}, \qquad [1.1]$$

for a determined value of $\langle k \rangle$. Thus, for finite N, the resulting $P(k)$ is the binomial distribution. On the other hand, in the limit $N \to \infty$, the degree distribution $P(k)$ converges to a Poisson distribution. In general, $\mathcal{G}_{N,p}$ is not a connected graph; the value $p_c = \frac{\log N}{N}$ is a percolation limit of the structure, that is, for $p > p_c$ the network becomes connected [ERD 59, NEW 10]. The Erdös–Rényi model is named after Paul Erdös, who made important contributions to mathematics and especially in graph theory, and Alfréd Rényi. They introduced this model in 1959 in [ERD 59]; this was the first work suggesting a method to generate random networks. It is a model where percolation phenomena arise and is currently one of the structures commonly used in the study of dynamical processes on networks [NEW 10, BAR 08b].

Another common structure with the small-world property is generated with the Watts–Strogatz model [NEW 10, WAT 98]. In order to obtain networks with a short average distance between nodes $\langle d\rangle$, this model consists of the relocation of edges at random starting from a regular network. The model for the case in which the initial network is a ring is defined by the following rules: we start with a ring with N nodes and lines are added to connect each node with its k nearby neighbors ($k/2-1$ to both sides of each node), then each node in the resulting structure has a degree k and to avoid a complete graph it is required that $N \gg k \gg \log N \gg 1$. From this regular network, the end of each line is relocated with a probability p. The relocation requires changing one end of the line in order to establish a connection with nodes that are not in the initial k neighbors and thus, on average, $pNk/2$ lines are relocated. The choice $p = 0$ results in a regular network, whereas for values $0 < p < 1$ the connections reduce the average distance $\langle d\rangle$. When $p = 1$, the resulting network is a disordered structure similar to the Erdös–Rényi random network. In Figure 1.4, we represent different cases of Watts–Strogatz networks with $N = 20$ nodes obtained for different rewiring probabilities p.

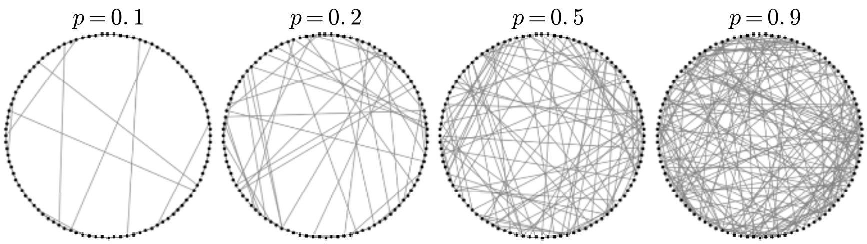

Figure 1.4. *Watts–Strogatz model. In this example, the initial network is a ring with $N = 20$ nodes. We add lines to connect each node to its two next neighbor's neighbor nodes, and the resulting structure has a constant degree $k = 4$. Then, for $0 < p < 1$ edges are randomly selected and one of its extremes is relocated. In the limit $p \to 1$, the network is similar to an Erdös–Rényi network*

The Watts–Strogatz model was introduced by Duncan J. Watts and Steven Strogatz in their joint paper [WAT 98] in 1998 in the context of synchronization in dynamical systems and was the first random graph model to explain how the small-world property emerges. In addition, the Watts–Strogatz model describes networks in which a large fraction of neighboring nodes are also connected. This feature is common in real networks, for example in the case of social networks a person can have many acquaintances who are friends with each other [WAT 98].

In addition to the networks described before, one of the most common networks in diverse applications is the random network generated by the Barabási–Albert model [NEW 10, BAR 99]. Through the implementation of this model a random network is generated, where the lines are added with a tendency to establish connections with higher degree nodes, and the resulting structure has a probability $P(k)$ of obtaining a node of degree k that follows a power-law relation for nodes with $k \gg 1$. In order to build the network, the algorithm starts with a number m_0 of fully connected nodes. At each step of the network growth, a new node is connected to m (with $m \leq m_0$) nodes in the network with a probability of connecting to a node i with degree k_i given by $p_i = k_i / \sum_{l=1}^{m} k_l$. This algorithm with a preferential attachment of links allows establishing a scale-free network with the small-world property. The Barabási–Albert model generates networks with a power law in the distribution of degrees of nodes. In these networks, there are a few nodes that have a large number of neighbors and a large number of nodes with few neighbors as we illustrate in Figure 1.5.

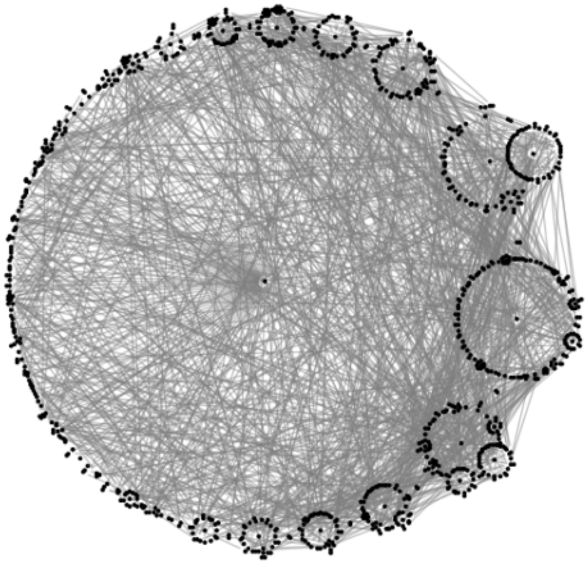

Figure 1.5. *Barabási–Albert random network with $N = 1,000$ nodes. We observe that there exists few nodes with a large number of connections and many nodes with few connections*

Finally, in addition to the artificial networks introduced in this section, it is worth mentioning that diverse real systems can be described by means of networks and the analysis of these has revealed structures with the small-world property. In particular, scale-free networks have been found in the context of the Internet structure, social networks that emerge in collaborations between scientists, online social networks, actors in Hollywood movies, transport networks, among countless real networks [NEW 10, COS 11]. Diverse characteristics of complex networks and how they emerge in real cases are studied in [NEW 10].

1.3. Spectral properties of the Laplacian matrix

The spectral analysis of diverse matrices associated with networks reveals structural properties and is an important tool in the study of dynamical processes taking place on networks [MIE 11, GOD 01]. In this section, we present some basic definitions and results about the Laplacian matrix of a simple undirected graph that describes the topology of a network. We also explore general properties related to the eigenvalues and eigenvectors of this matrix.

1.3.1. *Laplacian matrix*

We consider undirected simple connected networks with N nodes $i = 1, \dots, N$. The topology of the network is described by the adjacency matrix $\mathbf{A}$ with elements $A_{ij} = A_{ji} = 1$ if there is an edge (or link) between the nodes i and j and $A_{ij} = 0$ otherwise; in particular, $A_{ii} = 0$ avoiding links that connect a node with itself. In terms of the elements of the adjacency matrix, the degree k_i of the node i is the number of neighbors of this node and is given by $k_i = \sum_{l=1}^{N} A_{il}$. Now, by using this notation, the Laplacian matrix $\mathbf{L}$ of a network with N nodes is a symmetric $N \times N$ matrix with elements L_{ij} given by [NEW 10, GOD 01]

$$L_{ij} = k_i \delta_{ij} - A_{ij} \tag{1.2}$$

for $i, j = 1, 2, \dots, N$, where δ_{ij} denotes the Kronecker delta. In matrical representation we have $\mathbf{L} = \mathbf{K} - \mathbf{A}$, where we denote with $\mathbf{K}$ the diagonal matrix with the node degrees $k_1, k_2, \dots, k_N$ in the diagonal entries. In addition, from equation [1.2] we observe that non-diagonal elements of $\mathbf{L}$ are negative or null, and then $L_{ij} \leq 0$ for $i \neq j$.

On the other hand, one of the most important properties of the Laplacian matrix is that this matrix defines a quadratic form. In this way, for an arbitrary column vector $\mathbf{x}$ in $\mathbb{R}^N$ with components $x_1, x_2, \dots, x_N$, we have [GOD 01]

$$\mathbf{x}^T \mathbf{L}\, \mathbf{x} = \sum_{(i,j)\in\mathcal{E}} (x_i - x_j)^2 \geq 0, \tag{1.3}$$

where $\mathcal{E}$ denotes the set of edges of the network and the row vector $\mathbf{x}^T$ is the transpose of $\mathbf{x}$. The result in equation [1.3] implies that $\mathbf{L}$ is positive semidefinite.

EXAMPLE.– The Laplacian of an edge

In order to shed light on the general result in equation [1.3], it is convenient to analyze a simpler graph formed by the two nodes i and j connected with an edge $\epsilon = \{i, j\}$. In this case, the Laplacian matrix $\mathbf{L}_\epsilon$ is

$$\mathbf{L}_\epsilon = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \tag{1.4}$$

Hence, for a vector $\begin{bmatrix} x_i \\ x_j \end{bmatrix}$ we have

$$\begin{bmatrix} x_i & x_j \end{bmatrix} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} = (x_i - x_j)^2. \qquad [1.5]$$

Now, by using this result for the Laplacian of a general network $\mathbf{L}$ and the arbitrary column vector $\mathbf{x}$ in $\mathbb{R}^N$, we obtain

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \mathbf{x}^T \left[\sum_{\epsilon \in \mathcal{E}} \mathbf{L}_\epsilon \right] \mathbf{x} = \sum_{\epsilon \in \mathcal{E}} \mathbf{x}^T \mathbf{L}_\epsilon \mathbf{x}\,. \qquad [1.6]$$

Here, $\mathbf{L}_\epsilon$ is the $N \times N$ matrix associated with the edge $\{i, j\}$. The structure of this matrix $\mathbf{L}_\epsilon$ is similar to [1.4] but now described in terms of an $N \times N$ matrix. For this case, it is easy to show that the result in equation [1.5] is maintained and as a result, we have $\mathbf{x}^T \mathbf{L} \mathbf{x} = \sum_{\{i,j\} \in \mathcal{E}} (x_i - x_j)^2$, a relation that proves that the Laplacian is a quadratic form.

Going back to the general result in equation [1.3], this relation also can be deduced from the definition of the Laplacian matrix. By using this approach, we have

$$\begin{aligned} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} (x_i - x_j)^2 &= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} \left(x_i^2 + x_j^2 - 2 x_i x_j \right) \\ &= \frac{1}{2} \left(\sum_{i=1}^{N} 2 x_i^2 \underbrace{\sum_{j=1}^{N} A_{ij}}_{k_i} - 2 \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} x_i x_j \right), \end{aligned}$$

where the prefactor 2 in the first term of the last expression comes into play by using $A_{ij} = A_{ji}$, and this equation is then written as

$$\begin{aligned} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} (x_i - x_j)^2 &= \sum_{i=1}^{N} k_i x_i^2 - \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} x_i x_j \\ &= \sum_{i=1}^{N} \sum_{j=1}^{N} (k_i \delta_{ij} - A_{ij}) x_i x_j = \sum_{i=1}^{N} \sum_{j=1}^{N} L_{ij} x_i x_j . \end{aligned}$$

We can hence write equation [1.3] in the form of the last relation. In this way, the result in equation [1.3] implies that $\mathbf{L}$ is a positive semidefinite matrix and therefore its eigenvalues are all non-negative [GOD 01].

The Laplacian matrix contains all the information associated with the topology of a network and in this way is fundamental in the study of its characteristics as well as the analysis of dynamical processes taking place on networks. Diverse works have addressed this topic; in particular, the classic books of Godsil [GOD 01], Chung [CHU 97] and the recent work of Van Mieghem [MIE 11] review different aspects of algebraic graph theory and the spectra of networks. In the context of dynamical processes, properties of the Laplacian matrix have been explored in studies about synchronization and its relation with structural properties of networks [ARE 08], random walks and diffusion on networks and lattices [LOV 96, BLA 11, LAW 10], continuous-time quantum walks [MÜL 11], advanced techniques and algorithms for extracting useful information from network data [FOU 16], among many other processes [BAR 08b].

1.3.2. *General properties of the Laplacian eigenvalues and eigenvectors*

In this section, we present some general aspects related to the Laplacian matrix eigenvalues and the corresponding respective eigenvectors. Since $\mathbf{L}$ is a symmetric matrix, by using the Gram–Schmidt orthonormalization of the eigenvectors of $\mathbf{L}$, we obtain a set of eigenvectors $\{|\Psi_j\rangle\}_{j=1}^{N}$ that satisfies the eigenvalue equation[1]

$$\mathbf{L}\,|\Psi_j\rangle = \mu_j\,|\Psi_j\rangle\,, \qquad j = 1, \ldots, N. \tag{1.7}$$

In this relation, the eigenvalues of the Laplacian matrix are $\{\mu_j\}_{j=1}^{N}$ and as a direct consequence of the symmetry of $\mathbf{L}$ and the result in equation [1.3], the eigenvalues of $\mathbf{L}$ are real and non-negative. The set of eigenvalues is sorted in increasing order as follows:

$$0 \leq \mu_1 \leq \mu_2 \leq \mu_3 \leq \ldots \leq \mu_N. \tag{1.8}$$

On the other hand, for the set of eigenvectors, we have the orthonormalization condition[2]

$$\langle\Psi_i|\Psi_j\rangle = \delta_{ij}. \tag{1.9}$$

In addition, this set of eigenvectors satisfies the completeness relation

$$\sum_{l=1}^{N} |\Psi_l\rangle\,\langle\Psi_l| = \mathbf{I} \tag{1.10}$$

where $\mathbf{I}$ denotes the $N \times N$ identity matrix.

1 In various parts of the text, we use Dirac's notation for the eigenvectors of matrices.

2 Here, $\langle\Psi_i|$ denotes the Hermitian conjugate, denoted by $\dagger$, of the vector $|\Psi_i\rangle$. In this way, we have the relation $\langle\Psi_i| = [|\Psi_i\rangle]^{\dagger}$.

Now, once we have introduced the basic notation for the eigenvalues and eigenvectors of $\mathbf{L}$, the spectral form of the Laplacian is

$$\mathbf{L} = \sum_{m=1}^{N} \mu_m \left|\Psi_m\right\rangle \left\langle\Psi_m\right| . \qquad [1.11]$$

From this result we obtain for the trace (denoted as Tr$(\ldots)$) of the Laplacian matrix

$$\begin{aligned}\mathrm{Tr}(\mathbf{L}) &\equiv \sum_{i=1}^{N} L_{ii} = \sum_{i=1}^{N}\sum_{m=1}^{N} \mu_m \langle i|\Psi_m\rangle\langle\Psi_m|i\rangle \\ &= \sum_{m=1}^{N} \mu_m \langle\Psi_m| \left[\sum_{i=1}^{N} |i\rangle\langle i|\right] |\Psi_m\rangle = \sum_{m=1}^{N} \mu_m \langle\Psi_m|\Psi_m\rangle = \sum_{m=1}^{N} \mu_m.\end{aligned}$$

However, by using the definition of the Laplacian given by equation [1.2] we know that $\mathrm{Tr}(\mathbf{L}) = \sum_{i=1}^{N} k_i$, and consequently we obtain

$$\langle k\rangle = \frac{1}{N}\sum_{m=1}^{N} \mu_m, \qquad [1.12]$$

which is an invariant that relates the topology of the network with the eigenvalues of the Laplacian matrix where $\langle k\rangle = \frac{1}{N}\sum_{i=1}^{N} k_i$ is the average degree of the network.

On the other hand, from the definition in equation [1.2], the Laplacian satisfies

$$\sum_{j=1}^{N} L_{ij} = \sum_{j=1}^{N} k_i\delta_{ij} - \sum_{j=1}^{N} A_{ij} = k_i - k_i = 0. \qquad [1.13]$$

This relation in the elements of the Laplacian matrix introduces a restriction in the smallest eigenvalue of $\mathbf{L}$ and the respective eigenvector. In fact, the result in equation [1.13] requires

$$|\Psi_1\rangle = \frac{1}{\sqrt{N}}\begin{bmatrix} 1 \\ 1 \\ \ldots \\ 1 \end{bmatrix} \qquad [1.14]$$

and the corresponding eigenvalue is $\mu_1 = 0$. This is the lower bound of the Laplacian spectrum. In addition, the multiplicity of $\mu_1 = 0$, i.e. the number of eigenvalues with this value, is related to the connectivity of the network. In general, the multiplicity of the smallest eigenvalue of the Laplacian $\mathbf{L}$ is equal to the number of independent connected components in the network [MIE 11]. For a connected graph, $\mu_1 = 0$ is unique, thus

$$0 < \mu_2 \leq \mu_3 \ldots \leq \mu_N. \qquad [1.15]$$

The second smallest eigenvalue μ_2 gives us information about the connectivity of the graph. This quantity has been extensively explored in the context of partitioning of graphs [BIY 07]. Fiedler called μ_2 the *algebraic connectivity of a graph* [FIE 73], and the corresponding eigenvector $|\Psi_2\rangle$ is known as Fiedler vector [BIY 07]. For connected networks, the second smallest eigenvalue μ_2 satisfies [MIE 11]

$$0 < \mu_2 \leq \frac{N}{N-1} k_{\min}, \qquad [1.16]$$

where $k_{\min}$ denotes the minimum degree encountered in the network. The two smallest eigenvalues μ_1 and μ_2 of $\mathbf{L}$ are important in the study of dynamical properties of processes defined in terms of the Laplacian, and in a similar way the largest eigenvalue μ_N allows us to study particular asymptotic limits. The eigenvalue μ_N satisfies the inequality [MIE 11]

$$k_{\max} + 1 \leq \mu_N \leq \max\{N, 2k_{\max}\}; \qquad [1.17]$$

in this relation $k_{\max}$ is the largest degree of the nodes in the network.

1.3.3. *Spectra of some typical graphs*

In this section, we present the Laplacian spectra of particular types of networks. We explore three important networks: a complete graph, finite rings and interacting cycles. For these cases, the eigenvalues and eigenvectors of the respective Laplacian matrix can be obtained due to the fact that these structures are described by circulant matrices [MIE 11]. In this way, the eigenvectors of the Laplacian are Bloch vectors with the components $\langle l|\Psi_m\rangle = \frac{1}{\sqrt{N}}\zeta^{(l-1)(m-1)}$, where $\zeta = e^{-\mathrm{i}\frac{2\pi}{N}}$ with $\mathrm{i} = \sqrt{-1}$. In the following, we present the set of the respective unsorted eigenvalues of the Laplacian matrix.

– *Complete graph*: in this network, all nodes are connected, and then $A_{ij} = 1-\delta_{ij}$ and each node has degree $k = N-1$. The Laplacian spectrum is $\mu_1 = 0$ and

$$\mu_2 = \ldots = \mu_N = N. \qquad [1.18]$$

– *Ring*: this is a one-dimensional lattice with periodic boundary conditions, each node having degree $k = 2$. The unsorted eigenvalues of the Laplacian matrix are

$$\mu_m = 2 - 2\cos\left[\frac{2\pi(m-1)}{N}\right] \qquad \text{for} \quad m = 1, \ldots, N. \qquad [1.19]$$

– *Interacting cycles*: in this type of network, initially N nodes form a ring. Then each node is connected to its J left and J right nearest nodes; $2J$ is the degree of the resulting structure [MIE 11]. The value J is the interaction parameter, and in this network all the two nodes whose distance in the initial ring is smaller than or equal to J are connected by additional bonds. The Laplacian matrix of interacting cycles is circulant and its unsorted Laplacian spectrum is given by $\mu_1 = 0$ and

$$\mu_m = 2J + 1 - \frac{\sin\left[\frac{\pi}{N}(N-m+1)(2J+1)\right]}{\sin\left[\frac{\pi}{N}(N-m+1)\right]}, \qquad m = 2, \dots, N \quad [1.20]$$

which is briefly derived in section 1.6. In Figure 1.6, we present all the possible interacting cycles with $N = 13$ nodes; in particular, for $J = 1$ the resulting network is a ring, whereas for $N = 6$ we have a fully connected graph.

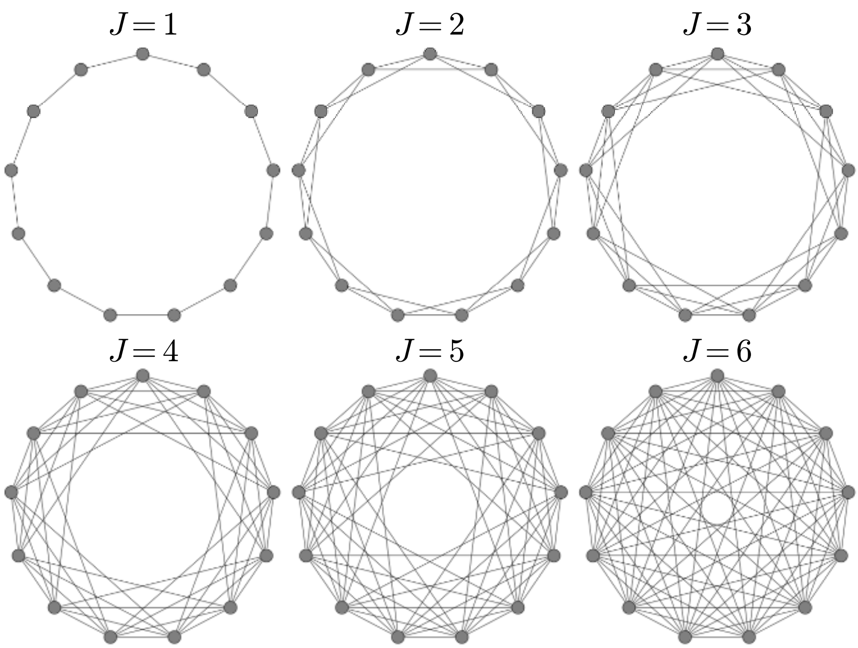

Figure 1.6. *Interacting cycles with $N = 13$ nodes. For $J = 1$, we obtain the initial ring; in this network, we add links in order to connect each node to its J left and J right nearest nodes. The value $J = 6$ defines a complete graph*

1.4. Functions that preserve the Laplacian structure

The objective of this section is to explore functions $g(\mathbf{L})$ of the Laplacian matrix in order to define new random walk strategies. From these functions, we can obtain new matrices that combine all the information of a network and for which emerge non-local correlations. We can use this non-locality to define quantities that describe the whole graph or to introduce new dynamical processes on networks.

1.4.1. *Function $g(\mathbf{L})$ and general conditions*

For a well-defined function $g(x)$ with $x \in \mathbb{R}$, the matrix $g(\mathbf{L})$ can be obtained by using the series expansion $g(x) = \sum_{n=0}^{\infty} c_n x^n$ or in terms of the spectral form of the Laplacian $\mathbf{L}$. For the second option, we have

$$g(\mathbf{L}) = \sum_{m=1}^{N} g(\mu_m) |\Psi_m\rangle\langle\Psi_m| \,. \qquad [1.21]$$

In the following, we denote as $g_{ij}(\mathbf{L})$ the i, j element of the matrix $g(\mathbf{L})$, and this notation is maintained for different functions of matrices explored in the rest of this chapter.

Although the result in equation [1.21] allows us to calculate general functions of the Laplacian, we are only interested in particular functions that preserve the *structure of the Laplacian matrix* described in section 1.3.2 and determined by the positive semidefiniteness of $\mathbf{L}$, the relation $\sum_{j=1}^{N} L_{ij} = 0$ and the property that all the non-diagonal elements satisfy $L_{ij} \leq 0$. As we will explore in Chapter 4, these conditions are necessary to define different random walk strategies on networks with transition probabilities between nodes expressed in terms of the function $g(\mathbf{L})$. In order to maintain these properties, we require that the function $g(\mathbf{L})$ satisfies the following conditions:

– *Condition I*: the matrix $g(\mathbf{L})$ must be positive semidefinite, i.e. the eigenvalues of $g(\mathbf{L})$ are restricted to be positive or zero.

– *Condition II*: the elements $g_{ij}(\mathbf{L})$, for $i, j = 1, 2, \dots, N$, should satisfy

$$\sum_{j=1}^{N} g_{ij}(\mathbf{L}) = 0. \qquad [1.22]$$

– *Condition III*: all the non-diagonal elements of $g(\mathbf{L})$ are non-positive and must satisfy $g_{ij}(\mathbf{L}) \leq 0$ where they are not allowed to be all simultaneously null, thus by condition II, equation [1.22], the diagonal elements $g_{ii}(\mathbf{L}) = -\sum_{j\neq i}^{N} g_{ij}(\mathbf{L}) > 0$ are all strictly positive.

The first condition is maintained if $g(x) \geq 0$ for $x \geq 0$, then $g(\mu_m) \geq 0$ for the values $m = 1, 2, \ldots, N$ and in this way the relations in equation [1.8] are also fulfilled by the eigenvalues of the matrix $g(\mathbf{L})$.

On the other hand, the second condition restricts the function $g(\mathbf{L})$ to preserve the particular property

$$\sum_{j=1}^{N} L_{ij} = 0$$

of the Laplacian matrix $\mathbf{L}$. As a direct consequence of this result, the Laplacian matrix has the eigenvector

$$|\Psi_1\rangle = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 \\ 1 \\ \ldots \\ 1 \end{bmatrix}$$

given in equation [1.14] and associated with the smallest eigenvalue $\mu_1 = 0$. In addition, the orthogonality condition $\langle \Psi_m | \Psi_1 \rangle = 0$ requires

$$\sum_{j=1}^{N} \langle \Psi_m | j \rangle = 0 \qquad \text{for} \quad m = 2, \ldots, N.$$

Then, by using the spectral form of $g(\mathbf{L})$ in equation [1.21], we have

$$\begin{aligned} \sum_{j=1}^{N} g_{ij}(\mathbf{L}) &= \sum_{j=1}^{N} \sum_{m=1}^{N} g(\mu_m) \langle i | \Psi_m \rangle \langle \Psi_m | j \rangle \\ &= \sum_{m=1}^{N} g(\mu_m) \langle i | \Psi_m \rangle \sum_{j=1}^{N} \langle \Psi_m | j \rangle, \end{aligned}$$

therefore

$$\sum_{j=1}^{N} g_{ij}(\mathbf{L}) = g(\mu_1) \langle i | \Psi_1 \rangle \sum_{j=1}^{N} \langle \Psi_1 | j \rangle = g(\mu_1) = 0. \qquad [1.23]$$

In this way, the condition II in equation [1.22] is fulfilled if the function $g(x)$ satisfies $g(0) = 0$.

Until now, we have determined the first two conditions for the function $g(\mathbf{L})$. However, these conditions are not at all sufficient to guarantee that $g(\mathbf{L})$ remains with all non-diagonal elements satisfying $g_{ij}(\mathbf{L}) \leq 0$ as this requires condition III. Before stating the main result, we illustrate this notion by giving an example.

EXAMPLE.– Functions of the Laplacian of a star graph

A star graph with N nodes is a tree for which one node is connected to $N - 1$ nodes. Then, in this structure we have a node with degree $k = N - 1$ and $N - 1$ nodes with degree $k = 1$. The Laplacian matrix for a star with $N = 5$ nodes is

$$\mathbf{L} = \begin{bmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{bmatrix}. \qquad [1.24]$$

In this case, the first node is connected to the rest of the network.

Now, we can verify that the function $G(x) = x^2$ fulfills the conditions $G(x) \geq 0$ for $x \geq 0$ and $G(0) = 0$. For this function, we have

$$\mathbf{L}^2 = \begin{bmatrix} 20 & -5 & -5 & -5 & -5 \\ -5 & 2 & 1 & 1 & 1 \\ -5 & 1 & 2 & 1 & 1 \\ -5 & 1 & 1 & 2 & 1 \\ -5 & 1 & 1 & 1 & 2 \end{bmatrix}. \qquad [1.25]$$

In this matrix, we can see how the function $G(\mathbf{L})$ satisfies conditions I and II; however, it fails in maintaining the required structure for non-diagonal elements of $G(\mathbf{L})$. On the other hand, for the function $F(x) = \log(1 + x)$, we obtain

$$\log(\mathbf{I} + \mathbf{L}) = \frac{1}{20} \begin{bmatrix} 16\log(6) & -4\log(6) & -4\log(6) & -4\log(6) & -4\log(6) \\ -4\log(6) & \log(196608) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) \\ -4\log(6) & -\log\left(\frac{16}{3}\right) & \log(196608) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) \\ -4\log(6) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) & \log(196608) & -\log\left(\frac{16}{3}\right) \\ -4\log(6) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) & -\log\left(\frac{16}{3}\right) & \log(196608) \end{bmatrix}.$$

Since the non-diagonal elements of $F(\mathbf{L})$ are negative, $F(x) \geq 0$ for $x \geq 0$ and $F(0) = 0$, we see that this function fulfills the conditions I–III required to maintain the structure of the Laplacian matrix.

1.4.2. *Non-negative symmetric matrices*

In this section, we explore the necessary conditions for an admissible class of functions $g(\mathbf{L})$ maintaining the condition III: $g_{ij}(\mathbf{L}) \leq 0$, for $i \neq j$. Then, let us consider the matrix $\mathbf{B}(t)$ given by

$$\begin{aligned} &\mathbf{B}(t) = \kappa\mathbf{I} - t\mathbf{L}, \\ &B_{ij}(t) = \delta_{ij}(\kappa - tk_i) + tA_{ij}. \end{aligned} \qquad [1.26]$$

Here, t is a real value in the interval $0 \leq t \leq 1$ and κ is a parameter that satisfies the condition $k_i \leq k_{\max} < \mu_N < \kappa$. The lower limit in the last inequality is determined by the condition in equation [1.17] for the largest eigenvalue μ_N. In the definition in equation [1.26], we observe that all matrix elements of $\mathbf{B}(t)$ are non-negative and satisfy $B_{ij}(t) \geq 0$ for t in the interval $0 \leq t \leq 1$; also, this condition is maintained for all the integer powers of $\mathbf{B}(t)$, i.e. $(\mathbf{B}^n)_{ij}(t) \geq 0$ for $n = 1, 2, 3 \ldots$.

On the other hand, from the spectral decomposition of the matrix $\mathbf{B}(t)$ in equation [1.26], we observe that

$$\mathbf{B}(t) = \sum_{m=1}^{N} (\kappa - t\mu_m)|\Psi_m\rangle\langle\Psi_m| \qquad [1.27]$$

is positive definite with eigenvalues $\kappa - t\mu_m > 0$ for $m = 1, 2, \ldots, N$ and $0 \leq t \leq 1$; in this way, positive definiteness is also preserved for all the integer powers of $\mathbf{B}(t)$:

$$f(x) = h(-x) > 0, \qquad x \geq 0 \qquad [1.28]$$

Now let be strictly positive over its interval of definition $0 \leq x < \infty$ where $x \geq 0$ includes the spectral interval $0 \leq \mu_m \leq \mu_N$ of the Laplacian eigenvalues. This corresponds to non-positive arguments $\xi = -x \leq 0$ as interval of definition for function $h(\xi = -x)$, thus

$$h(\xi) > 0, \qquad \xi \leq 0. \qquad [1.29]$$

We choose this positive scalar auxiliary function $h(\xi)$ such that it has only non-negative derivatives

$$h^{(n)}(\xi) = \frac{d^n}{d\xi^n} h(\xi) \geq 0 \qquad n = 1, 2, \ldots, \qquad \xi \leq 0. \qquad [1.30]$$

Now we consider the following matrix function that has, due to equation [1.29], uniquely positive eigenvalues $h(-t\mu_m) = h(-\kappa + \kappa - t\mu_m) > 0$, where $\kappa - t\mu_m > 0$, and expand this matrix, namely

$$h(-t\mathbf{L}) = h(-\kappa\mathbf{I} + \mathbf{B}(t)) = h(-\kappa)\mathbf{I} + \sum_{n=1}^{\infty} \frac{h^{(n)}(-\kappa)}{n!} (\kappa\mathbf{I} - t\mathbf{L})^n. \qquad [1.31]$$

We observe that each term in the series has only non-negative matrix elements since

$$\left[\frac{h^{(n)}(-\kappa)}{n!}(\kappa\mathbf{I} - t\mathbf{L})^n\right]_{ij} \geq 0 \qquad \text{for} \quad i,j = 1,\ldots,N \qquad [1.32]$$

has strictly non-negative matrix elements. Hence, it follows that $h(-t\mathbf{L}) = f(t\mathbf{L})$ is a matrix with strictly non-negative elements

$$h_{ij}(-t\mathbf{L}) = f_{ij}(t\mathbf{L}) \geq 0 \qquad \text{for} \quad i,j = 1,\ldots,N \quad \text{and} \quad 0 \leq t \leq 1 \qquad [1.33]$$

Now let us consider the integral for $0 \leq x \leq 1$

$$g(x\mathbf{L}) \equiv \int_0^x h(-t\mathbf{L})\mathbf{L}dt = -H(-t\mathbf{L})\Big|_0^x = H(0)\mathbf{I} - H(-x\mathbf{L}) \qquad [1.34]$$

where $H(\xi)$ denotes a primitive of $h(\xi)$ with $\frac{d}{d\xi}H(\xi) = h(\xi)$. We demonstrate now that the matrix function [1.34] indeed fulfills conditions I–III for good Laplacian matrix functions. The function $g(x)$ in equation [1.34] hence, by using equation [1.28], is constructed by the integral

$$g(x) = \int_0^x f(z)dz = \int_0^x h(-z)dz = H(0) - H(-x) \qquad x \geq 0 \qquad [1.35]$$

where according to equation [1.30] the functions $f(z) = h(-z)$ $(z \geq 0)$ have to satisfy

$$(-1)^n \frac{d^n}{dz^n} f(z) = \frac{d^n}{d\xi^n} h(\xi)\Big|_{\xi=-z} \geq 0, \qquad n = 1,2,.., \qquad z \geq 0, \qquad [1.36]$$

and as per the construction in equation [1.28] the function $g(x)$ has a *strictly positive non-vanishing derivative*

$$\frac{d}{dz}g(z) = f(z) = h(-z) > 0, \qquad [1.37]$$

i.e. $g(z)$ increases monotonously on the interval of definition $0 \leq z < \infty$. Especially due to the property $\frac{d}{dz}g(z)|_{z=0} = f(0) > 0$, the matrix function $g(\mathbf{L})$ has lowest order $\frac{d}{dz}g(z\mathbf{L})|_{z=0} = f(0)\mathbf{L}$ with positive non-zero coefficient $f(0)$. We observe by the monotonic increase in $g(z)$ from equation [1.37] that the so-constructed Laplacian matrix function $g(\mathbf{L})$ [1.21] *maintains the degrees of degeneracy* of the Laplacian eigenvalues since we have $g(\mu_m) > g(\mu_n)$ for $\mu_m > \mu_n$. The properties [1.28] with [1.36] and [1.37] guarantee that all coefficients in equation [1.31] are strictly non-negative. On the other hand, from equation [1.34] it follows that the first term in this relation $H_{ij}(0) = \delta_{ij}H(0)$ is diagonal. In this way, the off-diagonal elements in equation [1.34] are generated by the second term $-H(-x\mathbf{L})$, which has the expansion (where we set without loss of generality $x = 1$)

$$H(-\mathbf{L}) = H(-\kappa\mathbf{I}+\kappa\mathbf{I}-\mathbf{L}) = H(-\kappa)\mathbf{I}+\sum_{n=1}^{\infty}\frac{1}{n!}\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa}(\kappa\mathbf{I}-\mathbf{L})^n. \quad [1.38]$$

By accounting for equations [1.29] and [1.30], it follows that $\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa} \geq 0$, and thus the series occurring in equation [1.38]

$$\sum_{n=1}^{\infty}\frac{1}{n!}\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa}[(\kappa\mathbf{I}-\mathbf{L})^n]_{ij} \geq 0 \quad [1.39]$$

constitutes a matrix with strictly non-negative elements. Since this series generates the off-diagonal elements of $g(\mathbf{L})$, it follows that $g(\mathbf{L})$ has uniquely non-positive off-diagonal elements

$$\begin{aligned} g_{ij}(\mathbf{L}) &= [H(0) - H(-\mathbf{L})]_{ij} \\ &= (H(0) - H(-\kappa))\delta_{ij} - \sum_{n=1}^{\infty}\frac{1}{n!}\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa}[(\kappa\mathbf{I}-\mathbf{L})^n]_{ij} \\ &= -\sum_{n=1}^{\infty}\frac{1}{n!}\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa}[(\kappa\mathbf{I}-\mathbf{L})^n]_{ij} \leq 0 \qquad i \neq j. \end{aligned} \quad [1.40]$$

The Laplacian matrix function $g(\mathbf{L})$ of equation [1.34] hence fulfills condition III. In section 1.4.3 we demonstrate that $g(\mathbf{L})$ of equation [1.34] fulfills all conditions I–III of good Laplacian matrix functions.

1.4.3. *Completely monotonic functions*

From the results established above, we have shown that Laplacian matrix functions $g(\mathbf{L})$ that fulfill the necessary condition III are constructed by scalar functions in equation [1.35], namely

$$g(x) = H(0) - H(-x), \qquad 0 \leq x < \infty. \quad [1.41]$$

The function $g(x)$ can be expressed in terms of a function $f(x)$ that is defined on $0 \leq x < \infty$ and fulfills the following conditions

$$\frac{d}{dx}g(x) = f(x) > 0, \qquad 0 \leq x < \infty \quad [1.42]$$

as per the construction in equation [1.28] and further from equation [1.36], we have

$$(-1)^n\frac{d^n}{dx^n}f(x) \geq 0, \qquad 0 \leq x < \infty, \qquad n = 1, 2, \ldots \quad [1.43]$$

i.e. $\frac{d^n}{dx^n}f(x)$ have alternating signs if non-zero and where [1.42] is non-vanishing *positive* for $x \geq 0$, especially including the entire spectral interval $0 \leq x \leq \mu_N$ of the eigenvalues of the Laplacian matrix $\mathbf{L}$. A function $f(x)$ that fulfills the property [1.43] is referred to as *completely monotonic* [HAU 21]. As a result of equation [1.42], the function $g(x)$ is monotonously increasing in x. Some further consequences of equation [1.42] are worth mentioning. With the choice $\frac{d}{dx}g(x) = f(x) > 0$, the function $g(x)$ is *invertible* on its interval of definition $0 \leq x \leq \infty$, i.e. $x(g)$ exists (and constitutes also an admissible Laplacian function itself) having the interval of definition $0 \leq g < g_{max}$, where g_{max} may be finite or infinite. In a large network, the distance between two successive distinct Laplacian eigenvalues $\delta\mu_m = \mu_{m+1} - \mu_m << 1$ ($\mu_m < \mu_{m+1}$) becomes infinitesimal, namely $\delta g(\mu_m) = g(\mu_m + \delta\mu_m) - g(\mu_m) \approx f(\mu_m)\delta\mu_m$, thus the interval $\delta g(\mu_m) \sim \delta\mu_m$ between an eigenvalue and the next greater eigenvalue in equation [1.41] is of order $\delta\mu_m$ (multiplied with the positive (non-vanishing) scaling factor $f(\mu_m) > 0$). As mentioned, due to the monotonic increase in $g(\mu)$ in μ, the *degrees of degeneracy*[3] of the Laplacian eigenvalues μ_m are *maintained* in the matrix $g(\mathbf{L})$.

In addition, due to equation [1.35], the function $g(x)$ is then given by the following integral:

$$g(x) = \int_0^x f(z)\,dz, \qquad 0 \leq x < \infty \tag{1.44}$$

which is the primitive of $f(x)$ with $g(0) = 0$ and with $g(x) > 0$ for $x > 0$. We observe that the interval of definition of $g(x)$ is $0 \leq x < \infty$, which contains the spectral interval. This behavior preserves the unique eigenvalue 0 and the $N-1$ positive eigenvalues with their respective degrees of degeneracy in the matrix function $g(\mathbf{L})$. Let us demonstrate that relations [1.41]–[1.44] indeed are sufficient to generate a class of scalar C^{∞}-functions[4] $g(x)$ that define good Laplacian matrix functions $g(\mathbf{L})$ fulfilling conditions I–III.

Equations [1.42] and [1.43] indicate that $f(x)$ is a *positive and monotonously decreasing* function of x over the entire interval of its definition $0 \leq x < \infty$, which includes the spectral interval $0 \leq x \leq \mu_N = \max(\mu_m)$. This function can be written as $f(x) = h(-x)$ ($x \geq 0$), where $f(-x) = h(+x)$ ($x \leq 0$) is a *monotonously increasing* function in x as a result of equation [1.43]. Function $g(x)$ in

3 If there were distinct points x_0 in the spectral interval of the Laplacian eigenvalues with vanishing $f(x_0)$, then this would accumulate eigenvalues of $g(\mathbf{L})$ at these points x_0 and generate there singularities in the density of eigenvalues. If $\delta g(x_0) = f(x_0 + \delta\mu) \sim (\delta\mu)^n$ ($n > 1$), i.e. $\delta\mu(x_0) \sim [(\delta g)(x_0)]^{1/n}$, then the eigenvalue density of $g(\mathbf{L})$ at x_0 becomes $D_L(x_0)\frac{\delta\mu(x_0)}{(\delta\mu(x_0))^n} \sim \delta\mu^{-(n-1)} \sim [(\delta g)(x_0)]^{-(n-1)/n} \to \infty$. For instance, for $n = 2$, this would generate a $1/\sqrt{(\delta g)(x_0)}$-singularity (where $D_L(x_0)$ indicates the finite eigenvalue density of $\mathbf{L}$ at x_0).

4 C^{∞}-functions = infinitely often continuously differentiable functions.

equation [1.44] has the following general structure given in equation [1.41], and, in this way, admissible Laplacian matrix functions can be represented as

$$g(\mathbf{L}) = H(0)\mathbf{I} - H(-\mathbf{L}) = \sum_{m=2}^{N} (H(0) - H(-\mu_m)) |\Psi_m\rangle\langle\Psi_m| \qquad [1.45]$$

where we observe directly from equation [1.41] that *condition I*, namely $H(0) - H(-\mu_m) \geq 0$, is fulfilled (where $g(\mu_1 = 0) = H(0) - H(-\mu_1 = 0) = 0$ and $g(\mu_m) = H(0) - H(-\mu_m) > 0$ $(m = 2, \ldots, N)$).

In the canonic decomposition [1.45], there is no term $|\Psi_1\rangle\langle\Psi_1|$ since $g(\mu_1 = 0) = H(0) - H(-\mu_1 = 0) = 0$. The eigenvector $\langle i|\Psi_1\rangle = N^{-\frac{1}{2}}$ to the vanishing eigenvalue has identical components since the set of eigenvectors is conserved by matrix functions $g(\mathbf{L})$. It follows then that

$$0 = \langle i|g(\mathbf{L})|\Psi_1\rangle = \sum_{j=1}^{N}\langle i|g(\mathbf{L})|j\rangle\langle j|\Psi_1\rangle = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} g_{ij}(\mathbf{L}) \qquad [1.46]$$

which is indeed *condition II*. Furthermore, condition III was already demonstrated to be satisfied in above equation [1.40] since

$$H(-\mathbf{L}) = H(-\kappa\mathbf{I} + \mathbf{I}\kappa - \mathbf{L}) = H(-\kappa)\mathbf{I} + \sum_{n=1}^{\infty} \frac{1}{n!}\frac{d^n}{d\xi^n}H(\xi)\Big|_{\xi=-\kappa} (\mathbf{I}\kappa - \mathbf{L})^n$$

is a matrix with non-negative off-diagonal elements. Hence the necessary and sufficient conditions I–III are fulfilled for Laplacian matrix functions of equation [1.45] [RIA 18]. We will see in subsequent chapters that rescaling the Laplacian function $g(x)$ by a positive multiplier does not change the random walk dynamics; we can construct an equivalent renormalized good Laplacian function to equation [1.41], namely

$$g(x) = \frac{1}{f(0)} (H(0) - H(-x)) \qquad [1.47]$$

which has an expansion

$$\begin{aligned} g(x) &= x + \frac{1}{f(0)} \sum_{n=1}^{\infty} \frac{d^n}{dz^n} f(z)\Big|_{z=0} \frac{x^{n+1}}{(n+1)!} \\ &= x + \frac{1}{f(0)} \sum_{n=1}^{\infty} (-1)^n |f^{(n)}(0)| \frac{x^{n+1}}{(n+1)!} \end{aligned} \qquad [1.48]$$

starting with x *as lowest order* where we have utilized $\frac{d^{n+1}}{dz^{n+1}}g(z) = \frac{d^n}{dz^n}f(z)$ $(n = 0, 1, 2, ..)$. Everywhere in the above derivations we always anticipate absolute convergence of the expansion [1.48]. The renormalized Laplacian function of equation [1.47], since $f(0) > 0$, fulfills the conditions I–III, and is hence *physically* equivalent to equation [1.41]. Functions of the Laplacian matrix maintaining these conditions so far have been little explored. Michelitsch *et al.* have analyzed conditions I and II in connection with the non-locality generated by matrix functions in lattices [MIC 14a]. Micchelli and Willoughby [MIC 79] gave the conditions on a function f so that if the matrix $\mathbf{M}$ is symmetric and non-negative so is $f(\mathbf{M})$.

A function $f(x)$ defined on $x \geq 0$ is said to be *completely monotonic* if it has derivatives $f^{(n)}(x)$ for $n = 0, 1, 2, \ldots$ and $(-1)^n f^{(n)}(x) \geq 0$ for all $x > 0$. The notion of completely monotonic functions was introduced by Felix Hausdorff in 1921 [HAU 21]. Completely monotonic functions play an important role in probability theory [FEL 71, ALZ 02] and other fields. We also mention that functions with a completely monotonic derivative are referred to as *Bernstein functions* [BER 29, HAU 21] (and see the references therein). In view of equations [1.42] and [1.43], good Laplacian functions $g(x)$ refer to the class of Bernstein functions that fulfill $g(x = 0) = 0$ and which are monotonously increasing with strictly positive non-vanishing first derivative $\frac{d}{dx} g(x) = f(x) > 0$ for all $x \geq 0$. It follows that not all Bernstein functions are good Laplacian functions, but good Laplacian functions $g(x)$ are always Bernstein functions. Generally, Bernstein functions are allowed to be non-vanishing at $x = 0$ and may have pointwise vanishing first derivatives for instance at $x = 0$, whereas these two properties are forbidden for good Laplacian functions.

There exists several types of completely monotonic functions that in combination with the integral in equation [1.44] allow us to define functions $g(\mathbf{L})$ that maintain the Laplacian structure. In the following, we analyze the particular cases:

– The function $f(x) = (\beta + 1)x^{\beta}$ with $\beta \leq 0$ fulfills the condition in equation [1.36] for a completely monotonic function. Consequently, the integral in equation [1.44] allows us to obtain $g(x) = x^{\beta+1}$; however, the additional condition $g(x = 0) = 0$ requires $-1 < \beta \leq 0$. Therefore, the function

$$g(x) = x^{\gamma} \qquad \text{with} \quad 0 < \gamma \leq 1 \qquad [1.49]$$

maintains the structure of the Laplacian described in conditions I–III. In the following section, we will study this function in connection with the fractional Laplacian of a network explored in Chapter 2.

– For the completely monotonic function $f(x) = \frac{\alpha}{1+\alpha x}$ with $\alpha > 0$, by using the integral in equation [1.44], we have

$$g(x) = \log(1 + \alpha x) \qquad \text{with} \quad \alpha > 0. \qquad [1.50]$$

– Another completely monotonic function is determined by the exponential $f(x) = ae^{-ax}$ with $a > 0$ for which we see that equation [1.36] is satisfied. The corresponding function $g(x)$ that preserves the Laplacian structure is

$$g(x) = 1 - e^{-ax} \qquad \text{with} \quad a > 0. \tag{1.51}$$

Now, let us illustrate the results in our previous discussion by means of some simple examples.

EXAMPLE.– Functions $g(x)$ that preserve the Laplacian structure

In this example, we explore three particular cases that allow us to illustrate different functions of the Laplacian matrix.

1) Consider the function $f(x) = (\lambda - x)^n$ for $0 \leq x < \lambda$ with integer powers $n \in \mathbb{N}$ and $\lambda > \mu_N > 0$, which fulfill equations [1.42] and [1.43]. Then we obtain from equation [1.44]

$$g(x) = \int_0^x (\lambda - t)^n \mathrm{d}t = \frac{1}{(n+1)} \left(\lambda^{n+1} - (\lambda - x)^{n+1}\right). \tag{1.52}$$

In this result, we observe the necessary property that $g(x) > 0$ increases monotonously over the spectral interval $0 \leq x \leq \mu_N < \lambda$ (with monotonously decreasing positive derivative $f(x) > 0$). This gives the matrix function

$$\begin{aligned} g(\mathbf{L}) &= \frac{1}{(n+1)} \left(\lambda^{n+1}\mathbf{I} - (\lambda\mathbf{I} - \mathbf{L})^{n+1}\right) \\ &= \sum_{m=1}^{N} |\Psi_m\rangle\langle\Psi_m| \frac{1}{(n+1)} \left(\lambda^{n+1} - (\lambda - \mu_m)^{n+1}\right). \end{aligned} \tag{1.53}$$

We see that the first eigenvalue $g(\mu_1 = 0) = 0$ of [1.53] is vanishing preserving eigenvector $|\Psi_1\rangle$; these are properties I and II. This is guaranteed by $g(x = 0) = 0$ (relation [1.44]). In addition, because $\lambda > \mu_N \geq \mu_m$ in equation [1.53], the matrix $(\lambda\mathbf{I} - \mathbf{L})_{ij} \geq 0$ is a non-negative matrix. Hence as $\lambda^{n+1}\mathbf{I}$ is a diagonal matrix, the matrix function [1.53] fulfills property III, namely

$$g_{ij}(\mathbf{L}) \leq 0, \qquad \text{for} \qquad i \neq j. \tag{1.54}$$

Consider, for instance, the trivial case $n = 0$ that gives an admissible function $f(x) = 1$. Then $g(x) = x$ and this yields the trivial admissible case $g(\mathbf{L}) = \mathbf{L}$.

Now, when we explore the case $n = 1$, then $f(x) = \lambda - x$ where the positiveness of $f(x)$ over the spectrum of eigenvalues implies that only functions $\lambda - x$ are admissible with $\lambda > \mu_N$. Choosing such λ, we have from equation [1.44]

$$g(x) = \int_0^x (\lambda - t)\mathrm{d}t = -\frac{(\lambda - t)^2}{2}\bigg|_0^x = \frac{\lambda^2}{2} - \frac{(\lambda - x)^2}{2} \tag{1.55}$$

which gives the matrix function

$$g(\mathbf{L}) = \frac{\lambda^2}{2}\mathbf{I} - \frac{(\lambda\mathbf{I} - \mathbf{L})^2}{2} = \sum_{m=1}^{N} g(\mu_m)|\Psi_m\rangle\langle\Psi_m| \qquad [1.56]$$

with eigenvalues

$$g(\mu_m) = \frac{\lambda^2}{2} - \frac{(\lambda - \mu_m)^2}{2}, \qquad m = 1, 2, \ldots, N. \qquad [1.57]$$

Our first observation from equation [1.56] is, since $(\lambda\mathbf{I} - \mathbf{L})^2$ is a non-negative matrix and $\frac{\lambda^2}{2}\mathbf{I}$ is diagonal, that the non-diagonal elements are non-positive, i.e. $g_{ij}(\mathbf{L}) \leq 0$ for $i \neq j$, and second, from equation [1.57] it follows that the eigenvalue $g(\mu_1) = 0$ is vanishing since $\mu_1 = 0$, and further that all other $N - 1$ eigenvalues are positive, which is a direct consequence of the monotonousness of $f(-x) = x - \lambda$. As the vanishing eigenvalue $g(\mu_1) = 0$ refers to the same eigenvector $|\Psi_1\rangle$ as for $\mathbf{L}$, the conditions I and II are fulfilled.

2) In this second example, we consider $f(x) = \frac{1}{(1+x)^n}$ which is for $n \in \mathbb{N}$ an admissible function. The case $n = 1$ leads to the previously considered $g(x) = \log(1 + x)$ and let us explore here for simplicity $\mathbf{L}$ as the Laplacian of an edge given by

$$\mathbf{L} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \qquad [1.58]$$

The Laplacian of an edge has eigenvalues $\mu_1 = 0$ and $\mu_2 = 2$ which refer to the eigenvectors

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \qquad \text{and} \qquad |\Psi_2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

respectively. We have hence $\mathbf{L} = \mu_2|\Psi_2\rangle\langle\Psi_2|$, and

$$\begin{aligned} g(\mathbf{L}) = \log(\mathbf{I} + \mathbf{L}) = \log\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} &= |\Psi_2\rangle\langle\Psi_2|\log(1 + \mu_2) \\ &= \frac{1}{2}\begin{bmatrix} \log(3) & -\log(3) \\ -\log(3) & \log(3) \end{bmatrix}, \end{aligned} \qquad [1.59]$$

where again the zero eigenvalue is maintained for $m = 1$ and the second eigenvalue $\log(1 + \mu_2) = \log(3) > 0$. On the other hand, we see that the non-diagonal elements satisfy $g_{12} = g_{21} = -\frac{\log(3)}{2} < 0$ and in this way, all the required properties I–III are fulfilled.

Now, let us explore the cases with $n = 2, 3, \ldots \in \mathbb{N}, (n \neq 1)$. We have by the same procedure

$$g(x) = \frac{1}{(n-1)}\left[1 - \frac{1}{(1+x)^{n-1}}\right]$$

thus when $\mathbf{L}$ again is the Laplacian matrix of an edge given by equation [1.58]

$$\begin{aligned} g(\mathbf{L}) &= \frac{1}{(n-1)}\left[\mathbf{I} - (\mathbf{I}+\mathbf{L})^{-(n-1)}\right] \\ &= \frac{1}{(n-1)}\left[1 - \frac{1}{(1+\mu_2)^{n-1}}\right]|\Psi_2\rangle\langle\Psi_2|, \end{aligned} \qquad [1.60]$$

and considering that in this case $\mu_2 = 2$, we obtain

$$g(\mathbf{L}) = \begin{bmatrix} A_n & -A_n \\ -A_n & A_n \end{bmatrix}, \qquad A_n = \frac{1}{2(n-1)}\left[1 - \frac{1}{3^{n-1}}\right] > 0 \qquad [1.61]$$

where we easily verify validity of conditions I–III. For instance, for $n = 2$ we have $g(\mathbf{L}) = \mathbf{I} - (\mathbf{I}+\mathbf{L})^{-1} = (\mathbf{I}+\mathbf{L})^{-1}\mathbf{L}$, which yields $A_2 = \frac{1}{3}$ in equation [1.61].

3) Finally, in this third example we discuss the function $f(x) = \gamma\, x^{\gamma-1}$, which as we obtained before, according to equations [1.42] and [1.43] is an admissible function only for $0 < \gamma \leq 1$. This yields $g(x) = x^{\gamma}$ and in this way we obtain the *fractional Laplacian matrix*

$$g(\mathbf{L}) = \mathbf{L}^{\gamma}.$$

Now, by implementing the same approach as in the second example, we have for an edge with Laplacian matrix in equation [1.58]

$$g(\mathbf{L}) = \mathbf{L}^{\gamma} = \mu_2^{\gamma}|\Psi_2\rangle\langle\Psi_2| = \begin{bmatrix} 2^{\gamma-1} & -2^{\gamma-1} \\ -2^{\gamma-1} & 2^{\gamma-1} \end{bmatrix}. \qquad [1.62]$$

From this expression, we verify easily the validity of conditions I–III.

With the three examples explored before, we conclude this section about functions $g(\mathbf{L})$ that maintain the Laplacian structure. The formalism introduced in this section is general and can be applied to completely monotonic functions that once integrated to obtain $g(x)$ through equation [1.44] yield a general representation of the form of equation [1.41]. Other examples of completely monotonic functions are the modified Bessel function of the first kind, the Mittag Leffler function that appears in the context of fractional calculus, among many others [MIL 01]. In addition, combinations of completely monotonic functions produce other types of functions that again fulfill the condition in equation [1.43] (see details in [MIL 01, MER 14]).

1.5. General properties of $g(\mathbf{L})$

Once we have identified functions that maintain the structure of the Laplacian matrix $\mathbf{L}$, in this part we discuss some general properties of the matrix $g(\mathbf{L})$.

1.5.1. *Diagonal elements (generalized degree)*

As per construction, diagonal elements of the matrix $g(\mathbf{L})$ are necessarily positive and, in analogy with the Laplacian matrix $\mathbf{L}$, we denote the diagonal elements of $g(\mathbf{L})$ as the *generalized degree* associated with the function g as

$$\mathcal{K}_i \equiv g_{ii}(\mathbf{L}).$$

Now, as a direct consequence of equation [1.23] and the condition $g(0) = 0$, we have

$$0 = \sum_{j=1}^{N} g_{ij}(\mathbf{L}) = \mathcal{K}_i + \sum_{j \neq i} g_{ij}(\mathbf{L}) \qquad [1.63]$$

with $i = 1, 2, \ldots, N$. Therefore, the generalized degree $\mathcal{K}_i$ can be expressed as

$$\mathcal{K}_i = -\sum_{j \neq i} g_{ij}(\mathbf{L}). \qquad [1.64]$$

On the other hand, the average of the generalized degree is defined by

$$\langle \mathcal{K} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{K}_i = \frac{1}{N} \mathrm{Tr}(g(\mathbf{L})) = \frac{1}{N} \sum_{i=1}^{N} g(\mu_i), \qquad [1.65]$$

showing that $\langle \mathcal{K} \rangle$ can be calculated directly from the spectrum of the Laplacian matrix $\mathbf{L}$. In the general case, the degree $\mathcal{K}_i$ is a quantity that not only incorporates information on the nearest neighbors of i, but also includes information of the whole structure. This non-locality is explored in the following section.

1.5.2. *Functions $g(\mathbf{L})$ for regular graphs*

Now, in order to understand the structure of the matrix $g(\mathbf{L})$, we analyze the particular case of regular networks. For this type of structure, the degree k (number of connections that a node has) is a constant and the Laplacian matrix $\mathbf{L}$ takes the form

$$\mathbf{L} = k\mathbf{I} - \mathbf{A}. \qquad [1.66]$$

Furthermore, the series expansion of $g(x)$ is given by

$$g(x) = \sum_{l=1}^{\infty} c_l x^l, \qquad [1.67]$$

where the constants c_l for $l = 1, 2, \ldots$, are particular for each function $g(x)$. Now, in terms of the series expansion in equation [1.67], we obtain the following result for regular networks:

$$g(\mathbf{L}) = \sum_{l=1}^{\infty} c_l (k\mathbf{I} - \mathbf{A})^l = \sum_{l=1}^{\infty} c_l \sum_{m=0}^{l} \binom{l}{m} (k\mathbf{I})^{l-m} (-1)^m \mathbf{A}^m$$

$$= \sum_{l=1}^{\infty} \sum_{m=0}^{l} c_l \binom{l}{m} k^{l-m} (-1)^m \mathbf{A}^m. \qquad [1.68]$$

The result in equation [1.68] establishes a connection between the matrix $g(\mathbf{L})$ with the integer powers of the adjacency matrix $\mathbf{A}^m$ for $m = 1, 2, \ldots$ for which the element $(\mathbf{A}^m)_{ij}$ is the number of all the possible paths connecting the nodes i, j with m links [GOD 01]. In addition, the diagonal element $(\mathbf{A}^m)_{ii}$ is the number of closed paths with m links on the network that start in the node i and end in the same node [GOD 01]. In this way, equation [1.68] reveals how the functions $g(\mathbf{L})$ change the local character of the Laplacian matrix $\mathbf{L}$ to a long-range operator. The resulting matrix is appropriate to define a diversity of dynamical processes with non-local interactions on networks. These types of applications in the context of random walkers are discussed in Chapter 4.

1.5.3. *Locality and non-locality of $g(\mathbf{L})$ in the limit of large networks*

The following observation with respect to the admissible functions $g(\mathbf{L})$ appears noteworthy. For simple connected networks, let us briefly consider matrix functions defined by powers of $\mathbf{L}$, namely $g_\beta(\mathbf{L}) = \mathbf{L}^\beta$. As we saw above only power functions with exponents $0 < \beta \leq 1$ are admissible. Powers with $\beta > 1$ are not since they do not fulfill equation [1.43]. From this observation follows that admissible functions $g(x)$, which obey for small arguments (up to irrelevant positive multipliers)

$$g(x) \sim x^\gamma, \qquad x \to 0+, \qquad 0 < \gamma \leq 1 \qquad [1.69]$$

where for $\gamma = 1$ the representation of equation [1.47] is renormalized in such a way that it yields $g(x) \approx x$ for $x \to 0+$. The lowest order in the expansion of an admissible function $g(x)$ either starts with x, in which case we call this class *type (i) functions*, or the expression in equation [1.69] starts with x^γ for $0 < \gamma < 1$, in which case we call $g(x)$ a *type (ii) function*.

By introducing this classification, we can see that the expansion of $g(x)$, up to unimportant positive multipliers, for type (i) functions are of the form $g(x) = x + \tilde{g}(x)$, whereas type (ii) functions have expansions that write as $g(x) = x^\gamma + \tilde{g}(x)$ $(0 < \gamma < 1)$. The parts $\tilde{g}(x)$ contain only powers greater than 1 in case (i) and greater than γ in case (ii), respectively. The classes (i) and (ii) are the only two classes of functions that are admissible. In view of examples considered above, the functions $1 - e^{-x}$ and $\log(1 + \alpha x)$ are type (i) functions, whereas x^γ $(0 < \gamma < 1)$ is of type (ii).

In this way, the lowest power in the expansion of $g(\mathbf{L})$ determines the dominant asymptotic structure of sufficiently large networks $N \to \infty$. Consequently, functions

$$g(\mathbf{L}) = \mathbf{L} + \tilde{g}(\mathbf{L}) \qquad [1.70]$$

of type (i) contain an internal length-scale defined by the local information of Laplacian $\mathbf{L}$. This type of non-locality depends on that length scale and by increasing the size N of the network, the Laplacian functions of type (i) become quasi-local. In contrast, functions of type (ii) define a fractional type of non-locality with

$$g(\mathbf{L}) = \mathbf{L}^\gamma + \tilde{g}(\mathbf{L}) \qquad 0 < \gamma < 1, \qquad [1.71]$$

which becomes asymptotically scale-free (asymptotically self-similar) in the limit of large networks $N \to \infty$. As a result, the type (ii) asymptotic scale-free non-locality is maintained over all scales when increasing the network. The asymptotic scale-freeness wipes out in the limit of infinite networks any local information on $\mathbf{L}$ and in this sense is universal. We will see in Chapter 4 that type (ii) non-locality leads to asymptotic emergence of Lévy flights (anomalous diffusion) on large networks $N \to \infty$. The type (ii) non-locality due to its asymptotic scale-freeness cannot be "localized" as in case (i) by increasing the size N of the network. The type (ii) non-locality thus remains "stable" when increasing the size of the network. We conjecture that only type (ii) non-locality can maintain communication in dynamically growing complex networks such as living structures and time-evolving networks, whereas under type (i) non-locality far distant nodes become disconnected. Again we emphasize what we will show later in detail, namely that only these two classes of functions $g(\mathbf{L})$ type (i) and type (ii) constitute good functions to define random walks. For the asymptotic behavior of the walk emerging in the limit of an infinite network only the lowest orders are relevant, i.e. $\mathbf{L}$ for type (i) and $\mathbf{L}^\gamma$ $(0 < \gamma < 1)$ for type (ii) functions, respectively. The part $\tilde{g}(\mathbf{L})$ containing the higher orders in $\mathbf{L}$ becomes irrelevant in the infinite network limit.

The existence of the two asymptotic limits that define type (i) and (ii) functions for networks with very large N allows us to identify that in this case the locality is defined by the matrix $\mathbf{L}$ and non-locality is essentially dominated by the *fractional Laplacian* $\mathbf{L}^\gamma$ with $0 < \gamma < 1$. In this way, it is of utmost importance to understand the basic properties of this matrix and its non-local character. In Chapter 2, we will explore the fractional Laplacian of networks and in the second part of this book, we will explore this matrix in finite and infinite lattices as well as its connection with operators in fractional calculus. We will thoroughly analyze in Chapters 6–8, several aspects of the large network effects that emerge from walks generated by type (i) and type (ii) Laplacian matrix functions.

1.6. Appendix: Laplacian eigenvalues for interacting cycles

Let us briefly derive the eigenvalues of interacting cycles of equations [1.20]. Here, each node has connections to the J left and J right neighbors. Then the eigenvalues are obtained by

$$\begin{aligned}\mu_m = \mu(\kappa_m) &= \sum_{p=1}^{J}\left(2 - e^{i\kappa p} - e^{-i\kappa p}\right) \\ &= 2J - \sum_{p=1}^{J} e^{i\kappa p} - \sum_{p=-J}^{-1} e^{i\kappa p} = 2J + 1 - \sum_{p=-J}^{J} e^{i\kappa p} \\ &= 2J + 1 - e^{-i\kappa J}\sum_{p=0}^{2J} e^{i\kappa p} = 2J + 1 - e^{-i\kappa J}\,\frac{\left(1 - e^{i\kappa(2J+1)}\right)}{\left(1 - e^{i\kappa}\right)}\end{aligned} \qquad [1.72]$$

where we denote $\kappa = \kappa_m = \frac{2\pi}{N}(m-1)$ $(m = 1,..,N)$. Now we have

$$\begin{aligned}&e^{-i\kappa J}\frac{1 - e^{i\kappa(2J+1)}}{\left(1 - e^{i\kappa}\right)} = e^{-i\kappa J}\frac{e^{i\kappa(2J+1)/2}}{e^{i\kappa/2}}\frac{\left(e^{-i\kappa(2J+1)/2} - e^{i\kappa(2J+1)/2}\right)}{\left(e^{-i\kappa/2} - e^{i\kappa/2}\right)} \\ &= \frac{\left(e^{-i\kappa(2J+1)/2} - e^{i\kappa(2J+1)/2}\right)}{\left(e^{-i\kappa/2} - e^{i\kappa/2}\right)} = \frac{\sin\left[(2J+1)\kappa/2\right]}{\sin\left(\kappa/2\right)}, \qquad \kappa_m \neq 0.\end{aligned} \qquad [1.73]$$

Then with $\kappa_m/2 = \frac{\pi}{N}(m-1)$ we get for the eigenvalues [1.72]

$$\mu_m = 2J + 1 - \frac{\sin\left[(2J+1)\kappa_m/2\right]}{\sin\left(\kappa_m/2\right)} = 2J + 1 - \frac{\sin\left[\frac{\pi}{N}(m-1)(2J+1)\right]}{\sin\left[\frac{\pi}{N}(m-1)\right]} \qquad [1.74]$$

which holds for $\kappa_m \neq 0$, i.e. $m = 2,..,N$. Now we can rewrite equation [1.74] by using $\sin(x) = \sin(\pi - x)$ together with $\sin((2J+1)(\pi - x)) = \Im(e^{\pi i(2J+1)}e^{-i(2J+1)x}) = (-1)^{2J+1}\Im(e^{-i(2J+1)x})$ with $x = \kappa/2 = (m-1)\pi/N$ and get for equation [1.74] the representation of equation [1.20]

$$\mu_m = 2J + 1 - \frac{\sin\left[\frac{\pi}{N}(N-m+1)(2J+1)\right]}{\sin\left[\frac{\pi}{N}(N-m+1)\right]} > 0, \qquad m = 2,..,N \qquad [1.75]$$

for the non-vanishing eigenvalues and with $\mu_1 = \mu(\kappa_1 = 0) = 0$ which follows directly from equation [1.72].