Chapter 2
Complex Networks

Reports of the death of reductionism are greatly exaggerated. It is so ingrained in our thinking that if one day some magical force should make us all forget it, we would promptly have to reinvent it. The real worry is not with reductionism, which, as a paradigm and tool, is rather useful. It is necessary, but no longer sufficient.

[…] Indeed, forced by an imminent need to go beyond reductionism, a new network-based paradigm is emerging that is taking science by storm. It relies on datasets that are inherently incomplete and noisy. It builds on a set of sharp tools, developed during the past decade, that seem to be just as useful in search engines as in cell biology. It is making a real impact from science to industry. Along the way it points to a new way to handle a century-old problem: complexity.

Taken from the article by Albert-László Barabási, "The network takeover", *Nature Physics* **8**, 14–16 (2012).

This chapter contains known definitions and (a few novel) results from Network Theory. This thesis is based on the mathematical background, the concepts, the network characterisation methods, and the results we present here. Hence, this chapter constitutes the methods we use to address the problem of the transmission of energy and synchronisation in complex networks. Specifically, our results on the transmission of energy are based on the knowledge and understanding of the network structures where the energy is transmitted and our results on synchronisation are mainly based on the topological and functional way the dynamical units are interconnected to form a complex network.

2.1 Networks

From a mathematical point of view, the concepts of a graph or a network are interchangeable. However, *graphs* are usually used in mathematical jargon, representing the connections among the elements of a finite set, whereas *networks* are associated to physical models representing the inter-connectivity of units in a natural system.

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Consequently, we use the concept of graph in the Methods sections, as these sections constitute the mathematical background for our physical models, and the concept of networks in the Results sections, as these sections deal with the principles and solutions of our physical models. In any case, both concepts describe a complex web-like structure that exhibits a vast range of challenges for its understanding.

The classification, characterisation, and analysis of networks has gained increasing attention by members of the Physics community in recent years, as well as other major areas of Science. The reason is that it provides a unified approach to analysing many real-world systems considered as Complex Systems, i.e., a set of interacting dynamical systems. Trying to decipher what organising principles lie within these natural systems is an enormous challenge, both from the topological (the underlying network structure) and the dynamical (the collective behaviour) point of view. Here, we focus on the topological aspects of these systems by presenting the notions and results that are derived from Network Theory.

2.1.1 Notions and Definitions

Definition 2.1 A general **graph** [1–4] is a pair of sets $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$, such that $\mathcal{V} = \{v_1, \ldots, v_N\}$ is a set of N **nodes** (also known as vertices or points) and $\mathcal{E} = \{e_1, \ldots, e_M\}$ is a set of M **edges** (also known as links or branches).

A third condition is needed to define a graph properly: an *incidence relationship*. Namely, a subset of $\mathcal{V} \times \mathcal{E}$. An incidence relationship is required in order to specify if an edge is incident with either one node (Fig. 2.1a), in which case it is named *loop*, or more nodes. If every element of $\mathcal{E}$ is incident with two nodes (loops are absent) (Fig. 2.1b), and no two edges are incident with the same pair of vertices (multiple edges between nodes are absent) (Fig. 2.1c), then $\mathcal{G}$ is said to be a *strict graph* or simply, a *graph*. Consequently, $\mathcal{E}$ is a subset of the set of unordered pairs of nodes. Furthermore, if the *incidence relationship* imposes a direction in the adjacency of nodes (Fig. 2.1d), $\mathcal{G}$ is said to be a *directed graph* or simply a *digraph*, such as in

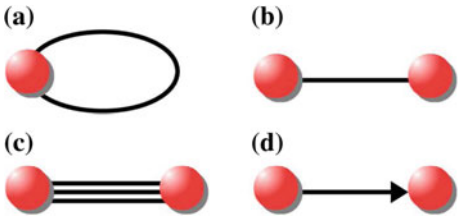

Fig. 2.1 Schematic representation of four different types of incidence relationships, namely, edges (*dark lines*) joining nodes (*filled circles*) in a graph. Panel **a** shows a loop, i.e., a self-edge, panel **b** shows an strict edge (or simply known as an edge), panel **c** shows multiple edges, and panel **d** shows a directed edge

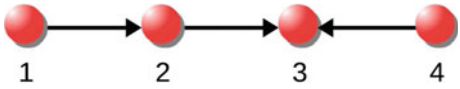

Fig. 2.2 Representation of a digraph with $N = 4$ nodes and $M = 3$ directed edges. The set of nodes is $\mathcal{V} = \{1, 2, 3, 4\}$ and the set of edges is $\mathcal{E} = \{\{1, 2\}, \{2, 3\}, \{3, 4\}\}$

Fig. 2.3 Representation of a strict connected graph with $N = 4$ vertices and $M = 3$ edges. The set of nodes and edges is identical to the sets in Fig. 2.2

Fig. 2.2. In what follows, unless otherwise stated, we focus solely on strict graphs, meaning that we exclude the possibility of having loops and/or multiple edges.

A third set $\mathcal{W}$ can be included in Definition 2.1 if weights are included to the edges connecting the nodes, namely, $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{W}\}$, where $\mathcal{W}$ is a set of numbers associated to each element of $\mathcal{E}$. In other words, the set $\mathcal{W}$ is a map, i.e., a one-to-one correspondence, from the domain of edges $\mathcal{E}$ to a co-domain of numbers, e.g., $\mathbb{R}^+$ (positive real numbers).

In particular, if we consider two nodes $v, w \in \mathcal{V}$ and an edge $e = \{v, w\} \in \mathcal{E}$, then e is said to *join* v and w (or that v and w are *adjacent*) and that these two elements are the *ends* of e [2]. The number of edges that v is an end, namely, the number of neighbours of v, is called the *degree of* v (or valency), d_v. For example, the degrees of the nodes in the line graph depicted in Fig. 2.3 are $d_1 = 1$, $d_2 = 2 = d_3$, and $d_4 = 1$. On the other hand, the node degrees of a digraph, such as the one depicted in Fig. 2.2, are split into in-degrees, $d_v^{(\text{in})}$, and out-degrees, $d_v^{(\text{out})}$. For example, in Fig. 2.2, the in-degrees and out-degrees of nodes 1 and 2 are $d_1^{(\text{in})} = 0 = d_3^{(\text{out})}$ and $d_1^{(\text{out})} = 1 = d_2^{(\text{in})}$.

We note that the concept of neighbouring nodes in a graph is purely topological. For example, two nodes representing two entities or systems that are physically far away (in the Euclidean metric sense), may be neighbouring nodes in the graph (in the topological sense) if there is an edge joining them, which can represent the interaction between the entities or systems. Namely, the edge joining the two nodes is simply stating that there is a connection between the two units.

Definition 2.2 A **path** of length L in a graph $\mathcal{G}$ [2] is defined by a sequence of node $(v_1, \ldots, v_{L+1}) \subset \mathcal{V}$ s.t. from each of its nodes, v_i, there is an edge $e_i \in \mathcal{E}$ that joins it to the next node in the sequence, v_{i+1}, for all $i = 1, \ldots, L$. If all nodes in the sequence are different, then the path is **elementary** (also known as simple).

We note that a path can be infinite, though a finite path always has a first node, known as the start node, and a final node, known as the end node. Both nodes are known as the terminal nodes of the path, whereas the remaining nodes are known as the internal nodes. For example, nodes 1 and 4 (nodes 2 and 3) are the terminal nodes

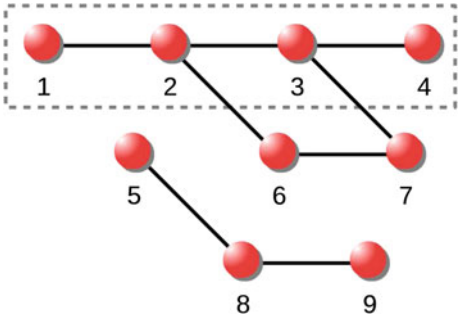

Fig. 2.4 Scheme of a graph with 2 connected components, namely, nodes {1, 2, 3, 4, 6, 7} and {5, 8, 9}. Within each connected component, any two nodes are joined by a path, such as the path between nodes 1 and 4, which is enclosed by the *dashed* line

(internal nodes) of the path that is identified by the dashed line in Fig. 2.4. Every node in a path is said to be *connected*, hence, a graph that contains only connected nodes is said to be a *connected graph*. We note that if a graph is not connected, as the graph in Fig. 2.4, it is known as a disconnected graph. This corresponds to having a set of nodes that is divided into subsets that are unreachable by any path trying to connect the subsets, such as the subset of nodes $\{1, 2, 3, 4, 6, 7\}$ and the subset of nodes $\{5, 8, 9\}$ in Fig. 2.4. This example shows that there are 2 connected components, where in each component the graph is connected.

In what follows, we choose to denote an elementary path as a path, reserving the notion of a *walk* for those cases where nodes in the sequence are repeated. For example, a walk in the graph of Fig. 2.4 is given by the sequence of nodes $(1, 2, 3, 7, 6, 2, 3)$. Moreover, in this thesis we deal with connected graphs alone, as any disconnected graph can be treated as a set of independent connected graphs. In other words, disconnected graphs are decomposable into connected components, hence, without loss of generality, their analysis is based on the separate connected components [3].

A path that includes every node in the graph (without repetition) is known as a *Hamiltonian path*. For example, Fig. 2.3 shows a connected strict graph where the sequence $(1, 2, 3, 4) \subset \mathcal{V}$ is a Hamiltonian path of length 3. Similarly, we can find a Hamiltonian path for the connected component, $\mathcal{S}_{\mathcal{V}} = \{1, 2, 3, 4, 6, 7\}$ of Fig. 2.4, for example, the Hamiltonian path with sequence $(1, 2, 6, 7, 3, 4)$. On the contrary, the connected digraph of Fig. 2.2 excludes any possible Hamiltonian path, as node 3 becomes an absorbing state for of any walk in the digraph. If the directed edge between nodes 3 and 4 was bidirectional, then, there is a directed Hamiltonian path that starts in node 1 and ends in node 4 passing through every node of the graph.

Another important concept related to paths is that of a *cycle*. A cycle is a (finite) path where the start and end node are the same (e.g., the line graph in Fig. 2.3 has no cycles). Consequently, the choice of a start node for a cycle is arbitrary. A cycle is said to be *elementary* (or simple) if a closed short-circuit is impossible and it is said to be a *Hamiltonian cycle* if it contains every node of the graph. We observe that both notions, paths and cycles, are extended to digraphs straightforwardly.

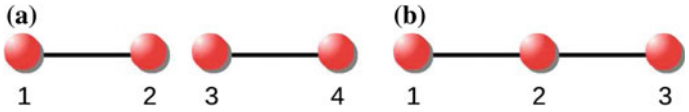

Fig. 2.5 Depiction of a sub-graph [panel (**a**)] and an induced sub-graph [panel (**b**)] that are derived from the line graph of Fig. 2.3 (the set of nodes for that line graph is: $\mathcal{V} = \{1,\ 2,\ 3,\ 4\}$)

Definition 2.3 A **sub-graph**, $\mathcal{S}_\mathcal{G}$, of a graph $\mathcal{G}$ is constructed by taking a subset, $\mathcal{S}_\mathcal{E}$, of $\mathcal{E}$ ($\mathcal{S}_\mathcal{E} \subset \mathcal{E}$) together with all the nodes incident, $\mathcal{S}_\mathcal{V}$, in $\mathcal{S}_\mathcal{E}$, resulting in a new graph $\mathcal{S}_\mathcal{G} = \{\mathcal{S}_\mathcal{V},\ \mathcal{S}_\mathcal{E}\}$.

Definition 2.4 An **induced sub-graph**, $\mathcal{U}_G$, of a graph $\mathcal{G}$ is obtained by taking a subset, $\mathcal{U}_\mathcal{V}$, of $\mathcal{V}$ ($\mathcal{U}_\mathcal{V} \subset \mathcal{V}$) together with all the edges which are incident in $\mathcal{G}$ and only contain nodes belonging to $\mathcal{U}_\mathcal{V}$.

For example, a sub-graph of the connected graph in Fig. 2.3 is constructed by selecting the edges $\mathcal{S}_\mathcal{E} = \{\{1,\ 2\},\ \{3,\ 4\}\} \subset \mathcal{E}$. Therefore, the resulting sub-graph is $\mathcal{S}_\mathcal{G} = \{\{1,\ 2,\ 3,\ 4\},\ \mathcal{S}_\mathcal{E}\}$, which has two connected components that are depicted in Fig. 2.5a. On the other hand, an induced sub-graph of the same graph $\mathcal{G}$ is generated by taking, for example, $\mathcal{U}_\mathcal{V} = \{1,\ 2,\ 3\}$, thus, $\mathcal{U}_G = \{\mathcal{U}_\mathcal{V},\ \{\{1,\ 2\},\ \{2,\ 3\}\}\}$, which is also a connected graph and is depicted in Fig. 2.5b.

2.1.2 Matrix Representations

The most common [1, 2], firstly used, and probably more intuitive matrix representations of a graph is the adjacency matrix.

Definition 2.5 The **adjacency matrix** of an unweighed graph $\mathcal{G}$ is the $N \times N$ representation, $\mathbf{A} = \mathbf{A}(\mathcal{G})$, whose entries are given by

$$A_{ij} = \begin{cases} 1, & \text{if nodes } v_i \text{ and } v_j \text{ are adjacent (i.e., } \{v_i,\ v_j\} \in \mathcal{E}), \\ 0, & \text{otherwise.} \end{cases}$$

It follows from Definition 2.5 that matrix $\mathbf{A}$ is symmetric ($\mathbf{A} = \mathbf{A}^T$, where T is the symbol corresponding to the transpose operation) if the graph is undirected, and that the trace of $\mathbf{A}$ is zero ($\text{tr}[\mathbf{A}] = 0$) if loops are absent. In the case of directed graphs, $\mathbf{A}$ is such that, if an edge from node i to j exists, then, $A_{ij} = 1$, but $A_{ji} = 0$. This indicates that there is no edge from node j to i. For example, the line digraph in Fig. 2.2 has an edge from node 1 to 2, but the edge from node 2 to 1 is absent. Hence, $A_{12} = 1$ and $A_{21} = A_{12}^T = 0$.

The topological *node degree*, $d_i \in \mathbb{N}$, of a node $i \in \mathcal{V}$ is the number of neighbours of node i. It is derived from $\mathbf{A}$ as

$$d_i = \sum_{j=1}^{N} A_{ij} = \left[\mathbf{A}\vec{1}\right]_i , \tag{2.1}$$

where $\vec{1} = (1, \ldots, 1)^T$ is the N-component column vector of unit entries. In the case that the graph is directed (the incidence relationship imposes a direction to the edges), then a *node in-degree*, $d_i^{(\text{in})}$, and a *node out-degree*, $d_i^{(\text{out})}$, are defined, which may differ in their values. Namely, there can be more or less edges that node i is an end than the edges that node i is a start. To compute their values we use the fact that the Adjacency matrix is such that $\mathbf{A} \neq \mathbf{A}^T$, as it holds the information of the incoming and outgoing edges for each node. Consequently,

$$d_i^{(\text{in})} = \sum_{j=1}^{N} A_{ji} = \left[\mathbf{A}^T\vec{1}\right]_i , \quad \text{and} \quad d_i^{(\text{out})} = \sum_{j=1}^{N} A_{ij} = \left[\mathbf{A}\vec{1}\right]_i . \tag{2.2}$$

In the most general scenario, a graph is also weighed. This means that there is another set $\mathcal{W}$ which is included in the definition of $\mathcal{G}$. The *weight set*, $\mathcal{W}$, associates a weight value to each edge in $\mathcal{E}$. Then, $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{W}\}$. In weighed graphs, the former definitions for node degrees are extended to their weighed versions straightforwardly. For example, the *weighted degree*, $dw_i \in \mathbb{R}$, of node $i \in \mathcal{V}$ is

$$dw_i = \sum_{j=1}^{N} W_{ij} = \left[\mathbf{W}\vec{1}\right]_i , \tag{2.3}$$

where W_{ij} is a symmetric weighted Adjacency matrix ($\mathbf{W} = \mathbf{W}^T$) for strict graphs that holds the adjacency information of the nodes and the weight of each of the edges. For the weighed digraphs, the weighted in-degrees and out-degrees are defined analogously as in Eq. (2.2) using $\mathbf{W}$ instead of $\mathbf{A}$.

We note that Eq. (2.1) defines a topological quantity. On the contrary, Eq. (2.3) defines a structural property because the result contains, not only the information of the topology, but also that of the weights. Hence, in this thesis, we will refer to structural quantities when the particular topology being analysed is weighed and refer to topological quantities when weights are absent.

Another matrix representation of the connectivity among the set of nodes, $\mathcal{V}$, which is often more useful for problems in Physics [3–7] and particularly useful for our work, is the Laplacian matrix, $\mathbf{G}$.

Definition 2.6 The **Laplacian matrix** of an unweighed graph $\mathcal{G}$ is the $N \times N$ matrix representation $\mathbf{G} = \mathbf{G}(\mathcal{G})$ whose entries are given by

$$G_{ij} = \begin{cases} d_i, & \text{if } i = j, \\ -1, & \text{if nodes } v_i \text{ and } v_j \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases}$$

It follows from the definition that matrix $\mathbf{G}$ is symmetric ($\mathbf{G} = \mathbf{G}^T$) if the graph is undirected, and that the trace of $\mathbf{G}$ is the sum of node degrees ($\text{tr}[\mathbf{G}] = \sum_{i=1}^{N} d_i$). In the case of directed graphs, two different Laplacian matrices are defined from the in-degrees and out-degrees of the nodes. In general, we can find a *Laplacian matrix* representation from

$$\mathbf{G} = \mathbf{D}_w - \mathbf{W}, \tag{2.4}$$

where $\mathbf{W}$ is the weighted adjacency matrix ($\mathbf{W} = \mathbf{A}$ for unweighed graphs and $\mathbf{W} = \mathbf{W}^T$ for undirected graphs with symmetric weights) and $\mathbf{D}_w$ is a diagonal matrix with entries given by the weighted node degrees ($[\mathbf{D}_w]_{ij} = \delta_{ij}\, dw_j$, where δ_{ij} is the Kronecker delta). Hence, in the case of directed graphs, the in-degree and out-degree Laplacian matrices are given by $\mathbf{G}^{(\text{in})} = \mathbf{D}_w^{(\text{in})} - \mathbf{W}^T$ and $\mathbf{G}^{(\text{out})} = \mathbf{D}_w^{(\text{out})} - \mathbf{W}$, respectively. In order to include loops, the node degrees diagonal matrix $\mathbf{D}_w$ adds the loop weight to its topological value, as this value appears in the diagonal of $\mathbf{W}$.

Definition 2.7 The **incidence matrix** of a connected graph $\mathcal{G}$ is the $N \times M$, with $N \leq M$ (where N is the number of nodes, and is also the necessary minimum number of edges, M, to have a connected graph), matrix representation $\mathbf{B} = \mathbf{B}(\mathcal{G})$ whose entries are given by

$$B_{ve} = \begin{cases} 1, & \text{if the edge } e \text{ enters node } v \text{ (node } v \text{ is the end of } e\text{)}, \\ -1, & \text{if the edge } e \text{ leaves node } v \text{ (node } v \text{ is the start of } e\text{)}, \\ 0, & \text{otherwise.} \end{cases}$$

It follows from Definition 2.7 that $\mathbf{B}$ is the relationship between the set of nodes $\mathcal{V}$ and the set of edges $\mathcal{E}$ [2]. In general, Definition (2.7) applies to graphs with loops, multiple edges, and even weights. However, in the weighed case, the incidence relationship $\mathbf{B}$ is maintained and weights are assigned by representing them in a separate diagonal matrix, $\mathbf{M}$, of $M \times M$ elements. The existence of matrix $\mathbf{M}$ is justified by the possibility of always defining an unweighed Laplacian matrix from the incidence matrix $\mathbf{B}$ alone, leaving the weights for separate analysis. In other words, we can always perform a topological analysis taking into account $\mathcal{E}$ alone, and another structural analysis taking into account $\mathcal{W}$. In particular, for strict graphs, the Laplacian matrix is found from the incidence matrix representation by

$$\mathbf{G} = \mathbf{B}\,\mathbf{B}^T. \tag{2.5}$$

The inclusion of weights in the derivation of the Laplacian matrix is done by using the diagonal $M \times M$ matrix of weights $\mathbf{M}$ as

$$\mathbf{G} = \mathbf{B}\,\mathbf{M}\,\mathbf{B}^T. \tag{2.6}$$

Hence, the effect of $\mathbf{M}$ is that of assigning the value of the square root of the weight associated to the entering and leaving edges instead of the 1 and -1 values in

Definition (2.7). In other words, the inclusion of **M** in Eq. (2.6) results in the same weighed Laplacian matrix as the one which is obtained from Eq. (2.5) if **B** is modified to include the square root of the edge weights.

These matrix representations of a graph are useful under different contexts. For example, some of our results on the synchronisation behaviour of networks of phase-oscillators depend on particular properties of the weighed adjacency matrix of those systems. Similarly, the incidence matrix representation of these systems is helpful to represent the diffusive coupling between the oscillators. On the same context, some of the Laplacian matrix properties are the ones determining if the system is able to achieve such collective behaviour. These results are found in Chap. 4.

2.1.3 Network Characterisation Methods

There are different characterisation methods that allow to classify graphs into separate groups [5–7]. For example, Fig. 2.6 shows 4 of the most common measures to differentiate between graphs. These are the node degree (signalled by the 3 dashed edges starting at node 8), clustering coefficient (found from the quantities within the rectangle, namely, the node degree and the dashed triangle), motifs (e.g., the trapeze and the angle signalled by the fine-dashed lines), communities (e.g., the decomposition of the graph into 2 modules linked by a hub node), and shortest-paths (diameter) (found from the minimization (maximization) of Definition 2.2).

The *node degree*, d_i, is the number of topological neighbours a node has. It is found from the adjacency matrix by Eq. (2.1). Hence, it is a local measure of the

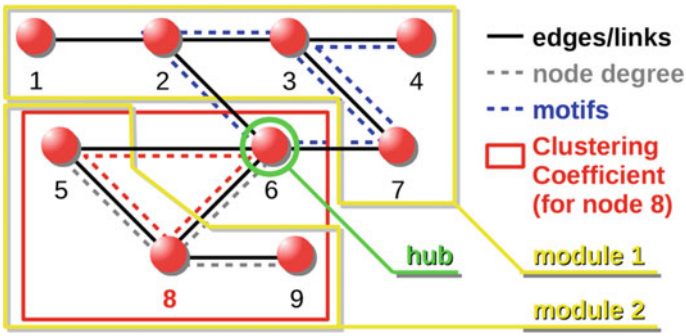

Fig. 2.6 Schematic representation of the following 4 characterisation measures for graphs. The node degree, which is signalled for node 8 by the dashed edges starting at the node (hence, $d_8 = 3$). The motifs of the graph, which two are signalled by fine-dashed lines, namely, a trapeze (nodes $\{2, 3, 6, 7\}$) and an angle (nodes $\{3, 4, 7\}$). The clustering coefficient, which for node 8 is $c_8 = 1/3$, is found from taking into account the nearest neighbours, i.e., the node degree, and the number of triangles formed with the neighbouring nodes (for node 8, this corresponds to the data enclosed within the rectangle that includes nodes $\{5, 6, 8, 9\}$). The community structure, which is signalled by the differentiation of 2 modules of nodes connected by a hub node (namely, node 6)

number of edges a node has. For example, node 8 in Fig. 2.6 has a degree $d_8 = 3$ and node 6 has the highest degree of the graph, $d_6 = 4$. The *average node degree* of a graph, $\langle d \rangle = \sum_{i=1}^{N} d_i/N$, is the global measure, although, from Eq. (2.1), we know that $\langle d \rangle = 2M$, which is simply twice the number of edges in the graph.

The local *clustering coefficient*, c_i, is a measure of how clustered the graph is. Specifically, it is a local measure of how many triangles a node has with its neighbours relative to the total possible amount of triangles it could have. Namely,

$$c_i = \frac{\left[\mathbf{A}^3\right]_{ii}}{d_i\,(d_i - 1)/2}, \tag{2.7}$$

where $[\mathbf{A}^3]_{ii}$ is the diagonal element of the third power of the adjacency matrix, which contains the number of triangles at node i, d_i is the degree of node i, and $d_i\,(d_i - 1)/2$ is the maximum number of triangles possible with d_i neighbours. For example, the clustering coefficient of node 8 in Fig. 2.6 is $c_8 = 1/3$, because $[\mathbf{A}^3]_{88} = 1$, $d_8 = 3$, and the maximum number of triangles possible for $d_8 = 3$ neighbours is 3. The *average clustering coefficient* of a graph, $\langle c \rangle = \sum_{i=1}^{N} c_i/N$, is a global measure.

The number of edges, measured by the node degree, and the number of triangles, measured by the clustering coefficient, are only two of the many possible motifs a graph can have. A *motif* is a subset of nodes that are strongly connected, i.e., they either have a Hamiltonian cycle or path joining them. For example, 3 nodes share a Hamiltonian cycle that forms a triangle or a Hamiltonian path that forms a line, as in the fine-dashed line in Fig. 2.6. However, as the number of nodes to be considered for a motif increases, the different possible motifs increases exponentially. Consequently, the search for motifs is usually performed only for the smaller motifs.

The path length is the topological distance between two nodes following some intermediate edges (see Definition 2.2). Hence, it is found from the adjacency matrix elements by summing the particular path. In particular, the *shortest-path length* between nodes i and j is

$$L_{ij} = \sum_{l=0}^{L^{\min}-1} A_{k_l,k_{l+1}} = A_{i,k_1} + A_{k_1,k_2} + \cdots + A_{k_{L^{\min}-1},j}, \tag{2.8}$$

where k_l, for $l = 1, \ldots, L^{\min} - 1$, indicates the interior nodes of the path which is subject to having the minimum value of L_{ij} by minimizing $L^{\min}$, and k_0 ($k_{L^{\min}}$) is node i (j). If L_{ij} is not a minimum, then L_{ij} is simply the distance between nodes i and j for a particular path. We note that, if in Eq. (2.8) instead of doing a minimization of the path length we do a maximization, then the result is the *diameter*, D, of the graph.

The *communities* of a graph is the decomposition of the graph into modules that have high intra-connectivity but low inter-connectivity. In other words, is a way to express the graph into sub-graphs (see Definition 2.3) that have many more edges within the modules than the edges inter-connecting the modules. Methods for

community detection, for example, look for the existence of hubs [8, 9] or for the maximisation of a modularity coefficient [10, 11]. Nevertheless, up to date, there is no general community detection method that is efficient for any topology [8–12]. In this thesis, we show how to use our exact solutions for the transmission of Energy in steady-state conservative flow-networks as a way to detect communities [13] (see Sect. 3.1.6).

2.1.4 Archetypal Networks

In graph theory there are some archetypal examples of graphs, such as the regular and tree graphs. These graphs are many times considered as the basic components in which to simplify and understand complex graph topologies, such as the relationship that the Kirchhoff's matrix-tree theorem [2] establishes between the number of spanning trees in any connected graph and its spectral characteristics.

A *tree graph*, $\mathcal{T}_N$, is an undirected graph without loops in which any two nodes are joined by exactly one path. In other words, any connected graph without simple cycles is a tree. In particular, a *star graph* $\mathcal{S}_N$ is a tree graph where every node is adjacent to a single (central) node. Namely, the central node has degree $N-1$ and all the remaining nodes have degree 1. A star graph and a tree graph of 6 nodes are depicted on the first and second diagrams of Fig. 2.7, respectively.

A *regular graph*, $\mathcal{R}_N$, is a strict graph of N nodes where each node has the same number of neighbours. In other words, every node has the same degree d, hence, the graph is usually called a d-regular graph (or a regular graph of degree d). In particular, the *complete graph*, $\mathcal{K}_N$, is the graph where every node is adjacent to every other node, namely, $\mathcal{K}_N$ is a $(N-1)$-regular graph. Another regular graph is the *ring graph* $\mathcal{C}_N$, which is a 2-regular graph made of a single Hamiltonian cycle. A complete graph and a ring graph of 6 nodes are depicted on the third and fourth diagrams of Fig. 2.7, respectively.

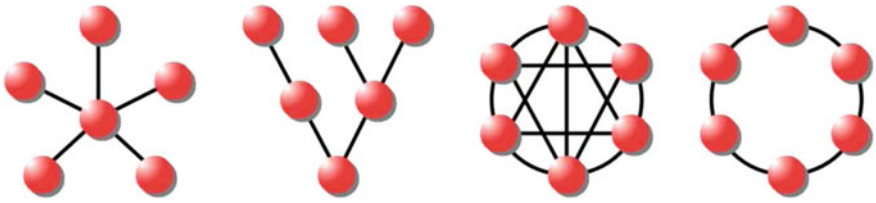

Fig. 2.7 Archetypal graphs of $N = 6$ nodes. From *left* to *right*, a star graph, a tree graph, a complete graph, and a ring graph, are shown

Circulant Graphs

In this work we take a special focus on *circulant graphs*. These graphs are such that a single line of their matrix representation is enough to fully characterise the graph. In particular, $\mathcal{R}_N$, $\mathcal{K}_N$, and $\mathcal{C}_N$ are all circulant graphs. The reason is that every line of its matrix representation is obtained by means of a cyclic permutation of any given reference line. For example, taking a ring graph of 3 nodes, $\mathcal{C}_3$ (which in this case is also a complete graph), its adjacency and Laplacian matrix are given by

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \tag{2.9}$$

We note that each row of $\mathbf{A}$ and $\mathbf{G}$ is a cyclic permutation of any reference row we consider. For example, taking the first row we have that $\mathbf{A} = \Pi_3[0,\ 1,\ 1]$ and $\mathbf{G} = \Pi_3[2,\ -1,\ -1]$, where Π_N is the set of N cyclic permutations, namely, $\Pi_N \equiv \{\pi^0, \pi^1, \pi^2, \ldots, \pi^{N-1}\}$, $\pi^0 \equiv \mathbf{I}$ being the identity operation and $\pi^1 \equiv \pi$ being the cyclic permutation matrix.

A *cyclic permutation*, π, in a 3-dimensional space is represented by

$$\pi = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \tag{2.10}$$

This means that when π is applied to, e.g., a column vector $\vec{v} = (x, y, z)^T$, the result is $\pi\,\vec{v} = (y, z, x)^T$, which is a cyclic permutation of the vector's elements. We note that the matrix representation of a clockwise cyclic permutation in any N-dimensional space requires a null diagonal and an immediately non-null upper diagonal (module N). The result of applying twice the matrix π of Eq. (2.10) to a vector, such as $\vec{v}$, is that

$$\pi \circ \pi\,\vec{v} = \pi^2\vec{v} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} z \\ x \\ y \end{pmatrix}.$$

Hence, π^2 is the cyclic permutation π applied two consecutive times. Consequently, the circulant matrix $\mathbf{A}$ and matrix $\mathbf{G}$ of Eq. (2.9) are found from applying the set $\Pi_3 = \{\mathbf{I}, \pi, \pi^2\}$ to the column vector $(0,\ 1,\ 1)^T$ as previously stated. Namely, $\Pi_3[0,\ 1,\ 1] \equiv \{\pi^0(0,\ 1,\ 1)^T,\ \pi^1(0,\ 1,\ 1)^T,\ \pi^2(0,\ 1,\ 1)^T\} = \mathbf{A}$ and $\Pi_3[2, -1, -1] \equiv \{\pi^0(2, -1, -1)^T,\ \pi^1(2, -1, -1)^T,\ \pi^2(2,\ -1, -1)^T\} = \mathbf{G}$, respectively. From a Group Theory point of view, Π_N is a modular Lie group representation of the finite cyclic group of permutations in N dimensions. For example, for Π_3, the set is modular because $\pi^3 = \mathbf{I} = \pi^0$. This means that any power of matrix π is expressed in terms of the powers of π up to order $N - 1$.

To summarise, a circulant graph is an undirected graph that has a cyclic group of symmetries, which includes the symmetry that takes any node to any other node (i.e., it includes $\mathbf{\Pi}_N$). Hence, all regular graphs are circulant. For circulant graphs, it is enough to know the incident connections to a single node of the graph to have the full graph connectivity. In other words, the graph looks exactly the same from any given node. This view-point is very similar to how a crystal lattice is defined in solid-state physics. There, the number of different crystalline structures is bounded by the number of symmetries of the space embedded, namely, the 14 Bravais lattices for a three-dimensional Euclidean space, which is also a consequence of the finite properties of the symmetry groups involved. Graphs, on the other hand, are not necessarily bounded by the metric space, hence, the number of different circulant graphs possible for a set of nodes is greater. The relevance of circulant graphs for this thesis goes beyond their simple matrix representation, and as it is seen in what follows (Sect. 2.3.2), it is linked to its spectral analysis.

Random Graphs

Another archetypal type of graph is the random graph. We can safely say that random graphs are the fruit fly of Graph Theory (the fruit fly is one of the most studied insects in Biology). Their quantitative characterisation was firstly done by P. Erdös and A. Rényi, and since their seminal paper [14] a vast amount of research has been devoted to understand all the properties that these graphs have.

A random graph is defined by a probability distribution of edges between a set of N nodes, $\mathcal{V}$, or by a random process that determines which nodes are adjacent. Hence, on the one hand we have a process that assigns equal probability of occurrence to all graphs that have exactly N nodes and M edges. On the other hand, we have a process that determines the set of edges, $\mathcal{E}$, by making a random choice of joining any two nodes of the set $\mathcal{V}$ with probability p independently (this process is the one depicted in Fig. 2.8). Both models are closely related and result in random graphs. These two processes are usually known as Erdös-Rényi graph (ERG) models.

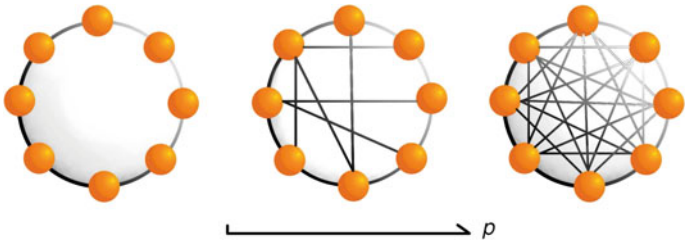

Fig. 2.8 Schematic representation of a random graph construction for a fixed set of nodes (*filled circles*) following Erdös-Rényi model. From *left* to *right*, the probability p of assigning an edge between a pair of nodes, considering every pair independently, is increased. Hence, for $p = 0$ the graph is disconnected, namely, the set of edges is empty ($\mathcal{E} = \varnothing$), and for $p = 1$ the graph is complete, namely, there is an all-to-all connectivity ($\mathcal{G} = \mathcal{K}_N$)

The process that assigns equal probabilities to all the random graphs with exactly $M \leq C \equiv N\,(N-1)/2$ edges, where C is the maximum number of edges possible for a graph with N nodes, has a probability distribution function (PDF), $G(N, M)$, with a probability of occurrence of $1/\binom{C}{M}$. For example, in the $G(3, 2)$ model (3 nodes and 2 edges) all three possible graphs are included (these are the three different line graphs that can be obtained from a set of ordered nodes) with probability 1/3. On the other hand, the construction that assigns a probability p to connect any pair of nodes from $\mathcal{V}$ determines a PDF, $G(N, p)$, that gives a probability of having a particular graph of M edges of $p^M\,(1-p)^{C-M}$. In particular, the expected number of edges, $E[M]$, for this ERG model, $G(N, p)$, is $p\binom{N}{2} = p\,C$ and the distribution of degrees for a particular value p is binomial. Namely, the probability of having a node with degree d is

$$P(d) = \binom{N-1}{d} p^d\,(1-p)^{N-1-d}, \tag{2.11}$$

hence, its limit for $N \to \infty$ and $N\,p = const.$ approaches a Poisson distribution, $(p\,N)^d\,e^{-p\,N}/d\,!$ The expected node degree for any case is $E[d] = p\,N$.

There are more properties that these graphs follow and have already been derived, however, our interest lies in their use. In particular, we focus on the second model of ERG, namely, the random process where we assign edges with a fixed probability p, with a slight modification [15] detailed in Sect. 3.1.4. The ERG model for random graphs construction constitutes a way to introduce heterogeneity and randomness into the topology of the connections between the dynamical units that compose our Complex Systems in a controlled way.

Small-World graphs

A Small-World graph (SWG) is a graph where most of the nodes are neighbours to each other, namely, the graph is approximately regular, although, most of the nodes are also reached by paths of small length, namely, $L \ll N$ (see Definition 2.2). Specifically, it is found that the typical distance, i.e., the expected path length $E[L]$, in SWGs between any two nodes of the graph chosen at random scales as $E[L] \propto \ln(N)$. This means that the resultant network is a small-world because the topological distance to reach a node from any other node is shorter than a regular graph or a ERG.

A certain class of SWG was identified as a type of random graphs by D. Watts and S. Strogatz in their seminal paper [16]. The particular identification of these graphs comes from the classification of generic random graphs according to their average clustering coefficient and average shortest-path length. They realised that these SWGs, although being random graphs in the general sense, have a smaller average shortest-path length and a significantly higher average clustering coefficient than the ERG models. The Strogatz-Watts graph (SWG) model for generating such graphs is depicted in Fig. 2.9. It is based on the randomisation of the edges of a regular graph by a process of rewiring. Specifically, each edge is rewired with a probability p,

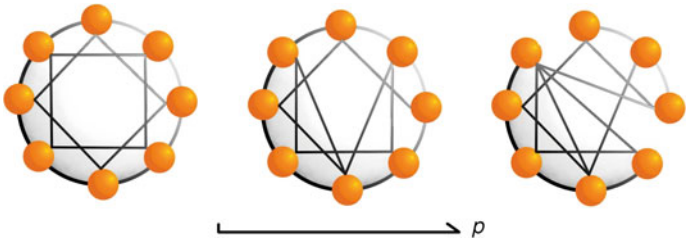

Fig. 2.9 Schematic representation of a small-world graph construction for a fixed set of nodes. From *left* to *right*, the probability p of rewiring an edge between a pair of nodes, considering every pair independently, is increased. Hence, for $p = 0$ the graph is regular ($\mathcal{G} = \mathcal{R}_N$), namely, the node degrees are all identical, and for $p = 1$ the graph is completely random

unless the rewired edge is another (existing) edge of the graph, then, the rewiring of that edge is undone. In particular, this is the process we follow in this thesis to generate SWGs.

2.2 The Laplacian Matrix

2.2.1 General Properties

As a consequence of Definition (2.6) and Eq. (2.4), *any Laplacian matrix fulfils a zero row sum* [3–5], regardless of its entry values,

$$\sum_{j=1}^{N} G_{ij} = \left[\mathbf{G}\vec{1}\right]_i = 0, \tag{2.12}$$

which means that the vector $\vec{1}$ belongs to the kernel of $\mathbf{G}$ ($\vec{1} \in \ker\{\mathbf{G}\}$). The kernel of a linear operator is the space of vectors that after the operation is carried the resultant vector is the null vector.

In general, a *Laplacian matrix of a graph $\mathcal{G}$ is a linear operator* on the space of functions f whose domain is the set of nodes $\mathcal{V}(\mathcal{G})$ [3]. Namely, the Laplacian matrix operation over a function $f : \mathcal{V}(\mathcal{G}) \to \mathbb{C}$ or $f : \mathcal{V}(\mathcal{G}) \to \mathbb{R}$ for complex or real-valued functions, respectively, satisfy

$$\mathbf{G}\, f(v_i) = \sum_{j=1}^{N} W_{ij}\, \left(f_i - f_j\right) = d_i\, f_i - \sum_{j=1}^{N} W_{ij}\, f_j. \tag{2.13}$$

where $f(v_i) = f_i$ [$f(v_j) = f_j$] is the value that the function takes at node v_i [v_j] and W_{ij} is ij th entry of the weighted adjacency matrix, which generates $\mathbf{G}$ by $\mathbf{G} = \mathbf{D} - \mathbf{W}$, $\mathbf{D}$ being the diagonal matrix of weighed node degrees.

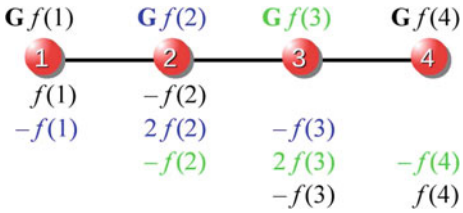

Fig. 2.10 Schematic diagram of how the Laplacian matrix, $\mathbf{G}$, of the line graph represented in Fig. 2.3, operates over a function $f : \{1, 2, 3, 4\} \to \mathbb{R}$

The form of Eq. (2.13) shows the similarity between the action of the Laplacian matrix in graph theory and the action of the Laplacian operator in differential geometry [3]. For instance, the Laplace equation of a function $f : D \subset \mathbb{R}^N \to \mathbb{R}$ is

$$\nabla^2 f(\vec{x}) = \sum_{i=1}^{N} \frac{\partial^2 f}{\partial x_i^2} = 0, \tag{2.14}$$

where $\left[\vec{x}\right]_i = x_i$ is a N-dimensional vector from the domain D and $\partial/\partial x_i$ is the partial derivative with respect to the coordinate x_i. In particular, for a 1-dimensional case, Eq. (2.14) has the following exact solutions for any point $x \in D$,

$$f(x) = \frac{1}{2}\left[f(x+h) + f(x-h)\right], \ \forall h > 0 \ \text{ s.t. } x+h \text{ and } x-h \in D. \tag{2.15}$$

These solutions are also verified by the one that is found from direct integration, namely, $f(x) = A\,x + B$, where A and B depend on the border conditions of D. Hence, the Laplace operator is always an averaging operation within the domain, holding $-f(x+h)+2f(x)-f(x-h)$ for the one dimensional case. This expression is identical to the result of applying $\mathbf{G}$ to a function f whose domain are the internal nodes of an unweighed line graph, such as the line graph in Fig. 2.3 taking $h = 1$. In that case, if x is node 2 (see Fig. 2.10), Eq. (2.13) holds

$$\mathbf{G}f(2) = d_2\, f(2) - \sum_{j=1}^{4} A_{2j}\, f(j) = 2f(2) - f(1) - f(3). \tag{2.16}$$

In general, any inner node of an unweighed line graph holds

$$\mathbf{G}f(i) = d_i\, f_i - \sum_{j=1}^{N} A_{ij}\, f_j = 2f_i - f_{i+1} - f_{i-1}. \tag{2.17}$$

These operations are also valid for complex valued ($\mathbb{C}$) functions. Consequently, the unweighed Laplacian matrix in graphs is an operation that compares evenly the function value at a node with the average of its values at the neighbouring nodes.

Definition 2.8 A matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ is said to be **non-negative**, in the element-wise sense, if all its entries are greater than or equal to zero, $\mathbf{A} \geq 0$, i.e., $A_{ij} \geq 0 \; \forall i, \; j$. It is called **positive** if the inequality is strict, i.e., $A_{ij} > 0 \; \forall i, \; j$.

Definition 2.9 A matrix is said to be **positive defined** (**positive semi-defined**), in the vectorial sense, if $\vec{v} \cdot \mathbf{A}\vec{v} = \vec{v}^T \, \mathbf{A} \, \vec{v} > 0 \, (\geq 0) \; \forall \vec{v}$.

As matrix multiplication preserves non-negativity if and only if the matrix is non-negative, these two definitions are related. However, from now on, we understand that non-negativity and positivity refers to the vectorial version (Definition 2.8), unless we explicitly state otherwise.

The *Dirichlet sum* of a function $f : \mathcal{V}(\mathcal{G}) \to \mathbb{R}$ is defined as [3]

$$f \cdot \mathbf{G} f = \sum_{i=1}^{N} f_i \sum_{j=1}^{N} G_{ij} f_j = \frac{1}{2} \sum_{i,\, j=1}^{N} W_{ij} \left(f_i - f_j \right)^2 \geq 0, \tag{2.18}$$

where "$\cdot$" represents the inner product operation (i.e., $\vec{x} \cdot \vec{y} = \sum_i x_i y_i^* = \vec{x}^T \vec{y}^*$ for complex-valued column vectors) and "$*$" denotes the complex conjugate operation. The appearance of the $1/2$ is due to the assumed symmetry in the edge weights and the inequality follows from the fact that the entries of matrix $\mathbf{W}$ are assumed as non-negative and real (which is the most common case for real world networks). This means that $\mathbf{G}$ is positive semi-defined in the matrix sense (Definition 2.9). In other situations, e.g., when $\mathbf{W}$ is non-symmetric, then the last equality in Eq. (2.18) changes and an explicit expression as a sum of binomial is impossible.

The *Rayleigh quotient* of a function $f : \mathcal{V}(\mathcal{G}) \to \mathbb{R}$ is defined as [3]

$$\frac{f \cdot \mathbf{G} f}{f \cdot f} = \frac{\sum_{i,\, j=1}^{N} \frac{W_{ij}}{2} \left(f_i - f_j \right)^2}{\sum_{i=1}^{N} f_i^2}. \tag{2.19}$$

In graph theory, both quantities are relevant for the computation of the spectrum of $\mathbf{G}$, namely, its eigenvalues and its eigenvectors [3].

2.2.2 Eigenvalues and Eigenvectors

Definition 2.10 The non-zero column vector $\vec{\psi}$ is said to be an **eigenvector** of matrix $\mathbf{A}$ if and only if

$$\mathbf{A} \, \vec{\psi} = \lambda \, \vec{\psi}, \tag{2.20}$$

where λ is a scalar value known as the **eigenvalue** of $\mathbf{A}$ corresponding to $\vec{\psi}$.

We note that Eq. (2.20) uses post-multiplication by vector $\vec{\psi}$, hence, it describes a right column-eigenvector of matrix $\mathbf{A}$. Using a pre-multiplication, the equation

describes a left row-eigenvector of $\mathbf{A}$, which may differ for some matrices. Definition 2.10 is non-restrictive in the matrix, eigenvalue, and eigenvector element values, allowing for all these quantities to take, for example, integer ($\mathbb{Z}$), real ($\mathbb{R}$), or complex ($\mathbb{C}$) values. We also note that the number of linearly independent vectors which fulfil Eq. (2.20) for a given λ determines the *geometric multiplicity*, $m_g(\lambda)$, of the associated subspace of λ. In other words, the dimension of the eigenspace associated to λ is $m_g(\lambda) \geq 1$. It is known that the different eigenspaces of $\mathbf{A}$, namely, the different eigenspaces corresponding to the different eigenvalues, form a direct sum. Consequently, their dimensions are strictly bounded by the dimension of $\mathbf{A}$.

These observations are derived from Eq. (2.20) in the following way. The *characteristic polynomial* $\chi(\lambda)$ of $\mathbf{A}$ is given by

$$(\mathbf{A} - \lambda\mathbf{I})\ \vec{\psi} = 0 \quad \Leftrightarrow \quad \chi(\lambda) \equiv \det(\mathbf{A} - \lambda\mathbf{I}) = 0, \tag{2.21}$$

where $\mathbf{I}$ is the identity matrix. The left hand side of Eq. (2.21) is the search for the scalar (λ) and vector ($\vec{\psi}$) quantities which fulfil Eq. (2.20). The right hand side of Eq. (2.21) is the restriction of matrix $\mathbf{A}-\lambda\mathbf{I}$ to have values that make it non-invertible, i.e., a matrix with null determinant. The polynomial $\chi(\lambda)$ encodes both requirements and provides all the eigenvalues of $\mathbf{A}$ by means of its roots. Hence,

$$\chi(\lambda) = \prod_{i=1}^{R} (\lambda_i - \lambda)^{m_a(\lambda_i)}, \tag{2.22}$$

R being the number of different roots of χ (namely, the different eigenvalues of $\mathbf{A}$), λ_i being the ith root of χ, and $m_a(\lambda_i)$ being the *algebraic multiplicity* of the ith eigenvalue (namely, the number of times the root appears in χ). We note that $\sum_{i=1}^{M} m_a(\lambda_i) = N$ always, where $N \times N$ is the dimension of matrix $\mathbf{A}$, and that only the roots λ_i are the scalar values able to fulfil Eq. (2.20) and simultaneously make $\mathbf{A} - \lambda\mathbf{I}$ non-invertible. Consequently, there are $R \leq N$ different subspaces that span the linear transformation $\mathbf{A}$. In order to find all the eigenvectors $\vec{\psi}_i$ belonging to each eigenspace, we need to solve the left hand side of Eq. (2.21) for each λ_i.

We distinguish between the subspaces corresponding to the non-zero eigenvalues ($\lambda \neq 0$), the *spanning eigenspaces*, and the subspace for the null eigenvalue ($\lambda = 0$), the *kernel eigenspace*. The set of linearly independent vectors that fall in the null vector, namely, $\mathbf{A}\vec{\psi} = \vec{0}$, conform the kernel of any linear transformation. The dimension of each subspace is given by their geometric multiplicity (the number of linearly independent eigenvectors corresponding to a given eigenvalue), which cannot exceed the algebraic multiplicity. Taking into account the spanning eigenspaces and the kernel, when the geometric multiplicities fulfil $\sum_{i=1}^{R} m_g(\lambda_i) = N$, there is a one-to-one correspondence with the algebraic multiplicities. In these cases, the matrix $\mathbf{A}$ is said to be *diagonalizable*. Furthermore, when the geometric and algebraic multiplicities are in one-to-one correspondence, the eigenvectors form a basis of vectors (they are spanning and linearly independent). Thus, they form an *eigenbasis*

for the vectorial space of $\mathbf{A}$. Consequently, the direct sum of eigenspaces equals the vectorial space where the linear transformation operates.

For *diagonalizable matrices* $\mathbf{A} \in \mathbb{M}_{N\times N}$ (real or complex valued), we have from Eq. (2.20), that

$$\mathbf{A}\,\mathbf{P} = \mathbf{P}\,\mathbf{\Lambda} \quad \Rightarrow \quad \mathbf{A} = \mathbf{P}\,\mathbf{\Lambda}\,\mathbf{P}^{-1}, \tag{2.23}$$

where $\mathbf{P} = \{\vec{\psi}_1, \ldots, \vec{\psi}_N\}$ is the change of basis matrix, $\mathbf{\Lambda} = \{\lambda_1, \ldots, \lambda_N\}$ is the eigenvalue diagonal matrix (with possible eigenvalue repetitions if any $m_a > 1$), and $\mathbf{P}^{-1}$ is the inverse of $\mathbf{P}$. These eigenvectors have the following properties

$$\begin{cases} \text{orthogonal: } \vec{\psi}_i \cdot \vec{\psi}_j = \sum_{k=1}^{N} \left[\vec{\psi}_i\right]_k \left[\vec{\psi}_j\right]_k^* = \delta_{ij}, \\ \text{normal:} \quad \left\|\vec{\psi}_i\right\|_2 = \sqrt{\vec{\psi}_i \cdot \vec{\psi}_i} = 1, \\ \text{complete:} \quad \sum_{k=1}^{N} [\mathbf{P}]_{ik} \left[\mathbf{P}^{-1}\right]_{kj} = \sum_{k=1}^{N} \left[\vec{\psi}_k\right]_i \left[\vec{\psi}_k\right]_j^* = \delta_{ij}, \end{cases} \tag{2.24}$$

where $[\vec{\psi}_i]_k$ is the kth component of the ith eigenvalue, "$\cdot$" is the inner product between vectors, "$*$" is the complex conjugate operation, and $\|\cdots\|_2$ is the Euclidean norm (also known as L_2-norm). The first two properties in Eq. (2.24) define the *orthonormal property* of the eigenvectors, which imply linear independence. The last property is the spanning condition of the eigenvectors, namely, that the set of eigenvectors forms a base for the vectorial space where $\mathbf{A}$ operates. The change of basis matrix, namely, $\mathbf{P}$, is said to be a *unitary* (*orthogonal*) *transformation* when the components of the eigenvectors are complex (real) numbers. Unitary (orthogonal) matrices fulfil $\mathbf{P}^{-1} = \mathbf{P}^{\dagger} \equiv \mathbf{P}^{*T}$ ($\mathbf{P}^{-1} = \mathbf{P}^{T}$), where † is the adjoint operation, ^{T} the transpose operation, and * the conjugate operation.

Definition 2.11 The **spectrum** of a graph, $\mathsf{Spec}(\mathcal{G})$, is the set of numbers which are eigenvalues of its matrix representation together with their multiplicities.

We observe that, if the distinct eigenvalues of $\mathbf{A}$ are $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_R$ and their corresponding multiplicities are $m\,(\lambda_1)$, $m\,(\lambda_2)$, $\ldots$, $m\,(\lambda_R)$, then, its spectrum is

$$\mathsf{Spec}(\mathbf{G}) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_R \\ m\,(\lambda_1) & m\,(\lambda_2) & \cdots & m\,(\lambda_R) \end{pmatrix},$$

with $\sum_{i=1}^{R} m\,(\lambda_i) = N$. In general, for connected strict graphs, the geometric multiplicities are identical to the corresponding algebraic multiplicities. However, even for the same graph, there is no general transformation that allows to obtain one spectrum from the knowledge of the spectrum of a different matrix representation.

2.2.3 Spectral Theorems

There are various important theorems about the spectral characteristics of matrices. Here, we enunciate a few of them which are particularly relevant for the study of transmission of Energy and Synchronisation in Complex Networks.

Theorem 2.1 *The eigenvalues of a Hermitian (real symmetric) matrix* $\mathbf{A}$*, i.e.,* $\mathbf{A} = \mathbf{A}^{*T} \equiv \mathbf{A}^{\dagger}$ $(\mathbf{A} = \mathbf{A}^{T})$*, are real and the eigenvectors form a complete eigenbase.*

Theorem 2.1 plays a major role in the study of graphs. In particular, the Adjacency and Laplacian matrix representations are symmetric for undirected graphs (see Sect. 2.1.2). Moreover, the only way these matrices have complex entries is when the weights associated to the edges are complex numbers, which is an unusual situation. As a consequence, *most graphs have a real spectrum and a real eigenbase of eigenvectors*. This guarantees that it is possible to express any function that operates in the set of nodes of the graph as a linear combination of the eigenvectors of the graph's matrix representation. The following Corollary is a straightforward application to graphs [2] of the two results of Theorem 2.1.

Corollary 2.2 *The spectrum of a strict unweighed graph is real and the multiplicity of each eigenvalue is equal to the dimension of the space of eigenvectors associated to it.*

In various situations we need approximate bounds for a graph's spectrum. In a similar way as Theorem 2.1 allows to know the characteristics of the spectrum values of a graph before solving the characteristic polynomial, the approximate bounds allow to know which are the possible spectrum minimum and maximum eigenvalue magnitudes before actually knowing them. In this sense, one of the most relevant theorems is the *Gershgorin Circle Theorem* [17]. The bounds that Theorem 2.3 imposes are valid even in the cases where the matrices are complex-valued.

Theorem 2.3 *(Gershgorin Circle) Given a matrix* $\mathbf{A} \in \mathbb{M}_{N\times N}$*, let* $\rho_i = \sum_{j\, j\neq i}^{N} \left|A_{ij}\right|$ *and* $D(A_{ii},\ \rho_i)$ *be the Gershgorin disk with centre at* A_{ii} *and radius* ρ_i*, then every eigenvalue of* $\mathbf{A}$ *lies within at least one of the Gershgorin disks.*

Consequently, the eigenvalues of any graph matrix representation are found within the Gershgorin disk that is centred at the minimum value of the diagonal elements and a radius that is obtained from the largest non-diagonal row sum. For example, the eigenvalues for the Laplacian matrix $\mathbf{G}$ of a strict graph are contained within the disk centred at $\min_{i\in\mathcal{G}}\{G_{ii}\} = \min(d)$ and with radius $\max_{i\in\mathcal{G}}\{\rho_i\} = \max(d)$, where $\min(d)$ $[\max(d)]$ is the minimum (maximum) node degree. In the case of strict graphs with positive weights, there is a more restrictive and precise result about the spectrum of the graph: the *Perron-Frobenius Theorem*.

Theorem 2.4 *(Perron-Frobenius) Let* $\mathbf{A}$ *be any real square non-negative matrix, then the following conditions are fulfilled.*

1. $\mathbf{A}$ *has a real non-negative characteristic root,* $\lambda_\rho \in \mathbb{R}^+$*, known as the* ***spectral radius*** *or* ***Perron root****, which is the largest eigenvalue of* $\mathbf{A}$ *in absolute value (i.e.,* $|\lambda_i| < \lambda_\rho$*, where* $i \neq \rho$*).*
2. *The spectral radius is a simple root of the characteristic polynomial* $\chi_{\mathbf{A}}$ *if* $\mathbf{A}$ *is positive, hence,* $m(\lambda_\rho) = 1$ *and* λ_ρ *is unique.*
3. *The eigenvector,* $\vec{\psi}_\rho$*, associated to* λ_ρ *is non-negative (i.e.,* $\mathbf{A}\,\vec{\psi}_\rho = \lambda_\rho\,\vec{\psi}_\rho$ *with* $[\vec{\psi}_\rho]_i > 0\ \forall\, i$*).*
4. *The remaining eigenvectors must have at least one negative or complex component.*
5. *The* ***Perron projection*** *is given by*

$$\lim_{n\to\infty} \frac{\mathbf{A}^n}{\lambda_\rho^n} = \vec{\psi}_\rho\,\vec{\phi}_\rho^{\,T}, \tag{2.25}$$

   where $\vec{\phi}_\rho$ *is the left row eigenvector associated to the spectral radius (*$\vec{\phi}_\rho\,\mathbf{A} = \vec{\phi}_\rho\,\lambda_\rho$*) and the result of the limit is a dyadic matrix between the eigenvectors (which are normalised to* $\vec{\phi}_\rho\,\vec{\psi}_\rho = 1$*).*
6. *The spectral radius satisfies the inequalities*

$$\min_i \left\{ \sum_{j=1}^{N} A_{ij} \right\} \leq \lambda_\rho \leq \max_i \left\{ \sum_{j=1}^{N} A_{ij} \right\}. \tag{2.26}$$

In general, the Laplacian matrix representation is the most convenient to formulate and analyse the transmission of Energy and Synchronisation in complex networks. This means that the matrix that are involved in the problem have non-positive off-diagonal elements. Hence, the Gershgorin Circle theorem is the one to provide the tools for the analytical study of the spectrum in these cases.

An important concept for the spectral characteristics of a matrix is its reducibility. In the cases where the matrix is reducible, its kernel has a non-null dimension. In other words, for a reducible matrix there are vectors that belong to the null eigenspace. Moreover, the number of linearly independent vectors that fall into the kernel space define its dimension. In general, the dimension of a matrix kernel space depends on the number of irreducible components in which the matrix can be decomposed. The reducibility is particularly important for Laplacian matrices [3] and the study of Random Walks [12] (see Sect. 3.1.6).

Definition 2.12 Let $\mathbf{A} \in \mathbb{M}_{N\times N}(\mathbb{R}) \geq 0$, then $\mathbf{A}$ is said to be **regular**, **indecomposable**, or **irreducible** if $\exists n \in \mathbb{N}$ such that for $n > 1$, $\mathbf{A}^n > 0$ (element-wise).

2.2.4 Spectral Properties of Laplacian Matrices

Since the rows and columns of the Adjacency and Laplacian matrices correspond to an arbitrary labelling of the nodes in graph $\mathcal{G}$, it is clear that properties that are invariant under permutations of rows and columns are the most relevant ones. Foremost among such properties are the spectral characteristics. Hence, we restrict ourselves to the study of the spectral properties of the matrix representation of the graph. In particular, to the Laplacian matrix $\mathbf{G}$. The study of the matrix $\mathbf{G}$ eigenvalues shows increasingly rich connections to almost all major invariants of a graph. We show here that the node degrees, clustering coefficients, and other methods that are commonly used to characterise graphs are related to the eigenvalues and eigenvectors of $\mathbf{G}$.

The smallest non-zero eigenvalue of a symmetric Laplacian $\mathbf{G}$, λ_2, is known as the spectral gap. In terms of the Rayleigh quotient [Eq. (2.19)], the spectral gap is found using $f = \vec{\psi}$ in Eq. (2.19) by [3]

$$\lambda_2(\mathbf{G}) = \inf_{\vec{\psi} \perp \vec{\psi}_1} \frac{\sum_{j=1}^{N} W_{ij} \left(\left[\vec{\psi} \right]_i - \left[\vec{\psi} \right]_j \right)^2}{2 \sum_{i=1}^{N} \left[\vec{\psi} \right]_i^2}, \tag{2.27}$$

where "inf" indicates that we take the infimum of the values that the quotient takes for different vectors $\vec{\psi}$ (in particular, the infimus is achieved if the eigenvector $\vec{\psi}_2$ is used), $\perp$ indicates that the infimus is sought for the orthogonal vectors with respect to the eigenvector $\vec{\psi}_1 = \vec{1}/\sqrt{N}$, which corresponds to $\lambda_1 = 0$, and W_{ij} is the symmetric and positive element-wise matrix of the network's representation. In general, the other eigenvalues ($n > 1$) are obtained similarly from

$$\lambda_n(\mathbf{G}) = \inf_{\vec{\psi} \perp \mathcal{P}_{n-1}} \frac{\sum_{j=1}^{N} W_{ij} \left(\left[\vec{\psi} \right]_i - \left[\vec{\psi} \right]_j \right)^2}{2 \sum_{i=1}^{N} \left[\vec{\psi} \right]_i^2}, \tag{2.28}$$

where $\mathcal{P}_{n-1}$ is the eigenspace spanned by the eigenvectors $\vec{\psi}_k$ corresponding to $k = 1, \ldots, n-1$. This means that the eigenvalues can be found directly from Eq. (2.28) by means of minimization techniques, without the need to find the roots of the characteristic polynomial, $\chi(\lambda)$, of Eq. (2.21).

The second smallest eigenvalue of a symmetric $\mathbf{G}$, λ_3, is known as the algebraic connectivity (or Fiedler value) of $\mathcal{G}$. These eigenvalues, and the largest eigenvalue, λ_N, are of major relevance in the Theory of Synchronisation. Furthermore, the spectral [Eq. (2.28)] in this case exhibits interesting analogies with the Spectral Riemannian Geometry and Stochastic Processes [3]. However, in this thesis we focus solely on the connections within Graph Theory.

We observe that Eqs. (2.27) and (2.28) assume a symmetric Laplacian matrix with positive semi-defined properties. In other words, the Laplacian matrix $\mathbf{G}$ is assumed to be derived from a non-negative matrix $\mathbf{W}$ ($W_{ij} \geq 0$ for all entries), namely, $\mathbf{G} = \mathbf{D} - \mathbf{W}$, where $\mathbf{D}$ is the diagonal matrix with entries given by $D_{ij} = \delta_{ij} \sum_{k=1}^{N} W_{jk}$. Consequently, these equations hold a positive spectra.

We note that, both the *determinant* and the *trace* of a matrix are invariant under cyclic permutation of their arguments [$\det(\mathbf{A}\,\mathbf{B}) = \det(\mathbf{B}\,\mathbf{A})$ and $\mathrm{tr}(\mathbf{A}\,\mathbf{B}) = \mathrm{tr}(\mathbf{B}\,\mathbf{A})$] and are invariant under changes of the labelling of nodes. Hence, considering a Laplacian matrix $\mathbf{G}$ of a weighed strict graph and the similarity transformation of Eq. (2.23), namely, the diagonalisation of $\mathbf{G}$, the determinant and trace of $\mathbf{G}$ are

$$\begin{cases} \det(\mathbf{G}) = \det\left(\mathbf{P}\,\mathbf{\Lambda}\,\mathbf{P}^{-1}\right) = \det(\mathbf{\Lambda}) \Rightarrow \det(\mathbf{G}) = \prod_{n=1}^{N} \lambda_n, \\ \mathrm{tr}(\mathbf{G}) = \mathrm{tr}\left(\mathbf{P}\,\mathbf{\Lambda}\,\mathbf{P}^{-1}\right) = \mathrm{tr}(\mathbf{\Lambda}) \qquad \Rightarrow \mathrm{tr}(\mathbf{G}) = \sum_{n=1}^{N} \lambda_n. \end{cases} \tag{2.29}$$

However, by Definition 2.6 and Eq. (2.4), $\mathbf{G} = \mathbf{D}_w - \mathbf{W}$, thus, the trace of the Laplacian is the sum of the node degrees as well: $\mathrm{tr}(\mathbf{G}) = \mathrm{tr}(\mathbf{D}_w) = \sum_i dw_i$. This means that

$$\mathrm{tr}(\mathbf{G}) = \sum_{n=1}^{N} \lambda_n = \sum_{i=1}^{N} dw_i. \tag{2.30}$$

Due to the zero row sum property ($\sum_j G_{ij} = 0\ \forall\, i$), any Laplacian matrix has a null eigenvalue with multiplicity given by the number of connected components of the graph [3]. As a result, $N \times N$ Laplacian matrices have a rank (i.e., the difference between the dimension of the space and the dimension of the kernel) less than N, $\mathrm{rank}(\mathbf{G}) < N$, which means that the matrix is reducible because it has at least one linearly dependent row. Another way to see this is that there is always an eigenvector $\vec{\psi}_1 = \vec{1}/\sqrt{N}$ (with unit L_2-norm) belonging to the kernel, i.e., corresponding to the eigenvalue $\lambda_1 = 0$, of each connected (irreducible) component of $\mathbf{G}$, such that,

$$\mathbf{G}\,\vec{\psi}_1 = 0\,\vec{\psi}_1 = \vec{0}. \tag{2.31}$$

Consequently, the determinant of a Laplacian matrix is always zero. Thus,

$$\det(\mathbf{G}) = \prod_{n=1}^{N} \lambda_n = 0. \tag{2.32}$$

Another consequence of having a non-empty kernel is that direct inversion is impossible. In particular, if $\mathbf{G}$ has a null eigenvalue with multiplicity R, we observe that $\mathbf{P}$ can be restricted to the N–R connected components (namely, the spanning subspaces), that the diagonal matrix $\mathbf{\Lambda}$ can be restricted to the $(N - R) \times (N - R)$

non-null eigenvalues, and the similarity condition of Eq. (2.23) still holds. Specifically, the entries of $\mathbf{G}$ in terms of its spectral decomposition are given by [13]

$$G_{ij} = \left[\mathbf{P}\,\mathbf{\Lambda}\,\mathbf{P}^{\dagger}\right]_{ij} = \sum_{k=1}^{N}\sum_{l=1}^{N}\left[\vec{\psi}_k\right]_i \delta_{kl}\lambda_l \left[\vec{\psi}_l\right]_j^* = \sum_{k=R+1}^{N}\left[\vec{\psi}_k\right]_i \lambda_k \left[\vec{\psi}_k\right]_j^* \quad \Rightarrow$$

$$\mathbf{G} = \mathbf{P}_R\,\mathbf{\Lambda}_R\,\mathbf{P}_R^{T*}, \tag{2.33}$$

where we assume that $\mathbf{P}$ is unitary, namely, $\mathbf{P}^{-1} = \mathbf{P}^{\dagger} = \mathbf{P}^{T*}$. The restricted spectral decomposition of the Laplacian matrix, Eq. (2.33), is the base for the construction of a pseudo-inverse Laplacian matrix [4] (Sect. 2.3.1).

In what follows we briefly derive a relationship between the eigenvalues and eigenvectors of the Laplacian matrix of a graph and the most common graph characterisation methods, namely, the node degree [Eq. (2.34)] and clustering coefficient [Eq. (2.35)]. These constitute novel relationships in the field of Network theory.

The *node degree distribution* of a connected strict graph is given by the distribution of the diagonal elements of its Laplacian matrix $\mathbf{G}$. Hence, by Eqs. (2.4) and (2.33), we have that the degree of node i, d_i, is given by

$$G_{ii} = d_i = \sum_{k=2}^{N}\lambda_k \left|\vec{\psi}_k\right|_i^2, \tag{2.34}$$

relating the node degree distribution with the spectra.

The *clustering coefficient distribution* of a connected strict graph is a measure of how many triangles exist for each node in the graph. It is found from

$$c_i = \frac{\left[\mathbf{A}^3\right]_{ii}}{d_i\,(d_i-1)/2}, \tag{2.35}$$

where $\mathbf{A}$ is the adjacency matrix of the graph. This means that Eq. (2.35) is a local measure quantifying the proportion of links between the nodes within the neighbourhood of node i divided by the number of links that could possibly exist between them, $d_i\,(d_i-1)/2$. Because $\mathbf{A} = \mathbf{D} - \mathbf{G}$, then Eq. (2.35) is related straightforwardly to Eqs. (2.33) and (2.34). Thus, a relationship between the local clustering coefficient and the graph invariants can be derived.

2.3 Resistance Distance

The *resistance distance* is a topological measure of the distance between two nodes in a network taking into account all the different paths that connect the two nodes [18–23]. Its name is related to that of the equivalent resistance (ER) in Circuit Theory.

The ER is a measure that is used in Circuit Theory to simplify the complexity of the circuit into simpler components by reducing the resistors in the network to a smaller set of equivalent resistors. The rules to obtain the ER are derived from the laws of Kirchhoff [24]. Using these laws, the ER between two points in the circuit is found by adding the resistors in series and inversely adding the resistors in parallel. However, this process requires planar graphs [2], hence, the resistance distance is an extension of this concept to any graph. In Graph Theory, the resistance distance for any graph topology is calculated using the spectral properties of its Laplacian matrix representation. Here, and as a consequence of both quantities holding identical values for planar graphs, we use them as synonyms.

2.3.1 Laplacian Matrix Pseudo-inverse

In order to derive an ER value for a generic network, we need to find the pseudo-inverse Laplacian matrix. As it was seen, particularly in Sect. 2.2.4, the Laplacian matrix is non-invertible due to the existence of at least one null eigenvalue ($\det[\mathbf{G}] = \prod_{n=1}^{N} \lambda_n = 0$). Hence, the search for a pseudo-inverse matrix. Namely, a Laplacian matrix $\mathbf{X}$ that when multiplied by the Laplacian matrix of the network $\mathbf{G}$ is approximately the identity matrix $\mathbf{I}$ [19].

We define the *pseudo-inverse Laplacian matrix*, $\mathbf{X}$, from the restriction of the eigenspace of the Laplacian matrix $\mathbf{G}$ [Eq. (2.33)] and define its elements by

$$X_{ij} \equiv \sum_{n=2}^{N} \left[\vec{\psi}_n\right]_i \frac{1}{\lambda_n} \left[\vec{\psi}_n\right]_j^*, \tag{2.36}$$

where $[\vec{\psi}_n]_i$ is the ith component for the nth eigenvector of the Laplacian matrix $\mathbf{G}$, namely, $\mathbf{G}\,\vec{\psi}_n = \lambda_n\,\vec{\psi}_n$, and the sum starts in $n = 2$ because we assume that the null eigenvalue is $\lambda_1 = 0$ with multiplicity 1. We note that if $\mathbf{G}$ is symmetric, then the eigenvalues and eigenvectors are real-valued. Hence, matrix $\mathbf{X}$ is also real-valued and the conjugate operation vanishes from Eq. (2.36). We interpret the definition of $\mathbf{X}$ by Eq. (2.36) as if the inverse operation of the Laplacian matrix would be performed in Eq. (2.33). The inversion would then act on the restricted diagonal matrix of eigenvalues by inverting them, although it would only act on the restricted eigenvector matrix as an adjoint operation (i.e., a transpose operation, ^{T}, plus a conjugate operation, *).

The first property of $\mathbf{X}$ [Eq. (2.36)] is that the zero-row-sum of a Laplacian matrix is fulfilled. Namely,

$$\mathbf{X}\,\vec{1} = 0, \tag{2.37}$$

which is found from observing that $\sum_{j=1}^{N} X_{ij} = \sum_{n=2}^{N} [\vec{\psi}_n]_i \frac{1}{\lambda_n} \sum_{j=1}^{N} [\vec{\psi}_n]_j^* = 0$ because $\sum_{j=1}^{N} [\vec{\psi}_n]_j^* = \sqrt{N} \vec{\psi}_1 \cdot \vec{\psi}_n$ for $n > 1$, where "$\cdot$" is the inner product, but from Eq. (2.24) this inner product is null ($\vec{\psi}_1 \cdot \vec{\psi}_n = 0 \; \forall \, n > 1$).

The second property of $\mathbf{X}$ is that it is itself a Laplacian matrix. The reason is that the diagonal terms, X_{ii}, are identical to the sum of the off-diagonal terms with opposite sign, i.e., $X_{ii} = -\sum_{j \neq i} X_{ij}$. Namely,

$$X_{ii} = \sum_{n=2}^{N} \frac{\left| \left[\vec{\psi}_n \right]_i \right|^2}{\lambda_n} = -\sum_{n=2}^{N} \frac{\left[\vec{\psi}_n \right]_i}{\lambda_n} \sum_{j \neq i}^{N} \left[\vec{\psi}_n \right]_j^* = -\sum_{j \neq i} X_{ij}. \tag{2.38}$$

The derivation of Eq. (2.38) is done by observing that $\sum_{j=1}^{N} [\vec{\psi}_n]_j^* = 0$ for $n > 1$, hence, $[\vec{\psi}_n]_i^* = -\sum_{j \neq i} [\vec{\psi}_n]_j^*$. Consequently, $\mathbf{X}$ behaves as a Laplacian matrix which posses a null eigenvalue with associated eigenvector $\vec{\psi}_1 = \vec{1}/\sqrt{N}$.

The third property is being the pseudo-inverse of Laplacian matrix $\mathbf{G}$. Namely,

$$\begin{aligned} [\mathbf{X}\,\mathbf{G}]_{ij} &= \sum_{n=2}^{N} \left[\vec{\psi}_n \right]_i \frac{1}{\lambda_n} \sum_{l=1}^{N} \left[\vec{\psi}_n \right]_l^* \sum_{m=2}^{N} \left[\vec{\psi}_m \right]_l \lambda_m \left[\vec{\psi}_m \right]_j^* \\ &= \sum_{n=2}^{N} \sum_{m=2}^{N} \left[\vec{\psi}_n \right]_i \frac{1}{\lambda_n} \left(\sum_{l=1}^{N} \left[\vec{\psi}_n \right]_l^* \left[\vec{\psi}_m \right]_l \right) \lambda_m \left[\vec{\psi}_m \right]_j^* = \sum_{n=2}^{N} \left[\vec{\psi}_n \right]_i \left[\vec{\psi}_n \right]_j^*, \end{aligned}$$

where the last equality is obtained from observing that $\sum_{l=1}^{N} [\vec{\psi}_n]_l^* [\vec{\psi}_m]_l = \delta_{nm}$. Moreover, because $\sum_{n=1}^{N} [\vec{\psi}_n]_i \, [\vec{\psi}_n]_j^* = \delta_{ij}$ [Eq. (2.24)] and for $n = 1$ we have $[\vec{\psi}_n]_i = 1/\sqrt{N}$ for all coordinates, then,

$$\mathbf{X}\,\mathbf{G} = \mathbf{I} - \frac{1}{N}\mathbf{J}, \tag{2.39}$$

where $I_{ij} = \delta_{ij}$ and $J_{ij} = 1$ for all i, j. Equation (2.39) is the demonstration that $\mathbf{X}$ is the pseudo-inverse of $\mathbf{G}$, and vice-versa [19]. Namely, $\mathbf{G}\,\mathbf{X} = \mathbf{I} - \frac{1}{N}\mathbf{J}$, hence, $[\mathbf{G}, \mathbf{X}] = 0$, which implies that these matrix commute.

The implication of the commutation relationship between $\mathbf{G}$ and $\mathbf{X}$, is that both matrix share a common set of eigenvectors. This is obvious from the definition of $\mathbf{X}$ as well. The difference lies in the eigenvalues of these matrix. While the eigenvalues of $\mathbf{G}$ are given by $\{\lambda_1 = 0, \, \lambda_2, \, \ldots, \, \lambda_N\}$, the eigenvalues of $\mathbf{X}$ are given by $\{\lambda_1 = 0, \, 1/\lambda_2, \, \ldots, \, 1/\lambda_N\}$.

For example, the Laplacian matrix of a complete graph $\mathcal{K}_N$ is $\mathbf{G} = N\,\mathbf{I} - \mathbf{J}$, with a set of eigenvalues given by $\lambda_1 = 0$ and $\lambda_k = N$ for all $k > 1$. Consequently, using $\mathbf{I}/N$ as a pseudo-inverse for $\mathbf{G}$ we fulfil Eq. (2.39). However, neither Eq. (2.37) nor Eq. (2.38) are fulfilled. Hence, the definition of $\mathbf{X}$ in Eq. (2.37) needs to be used to

calculate exactly the entries of the pseudo-inverse (this case is revisited in Sect. 2.3.2 to provide an explicit analytical expression for $\mathbf{X}$).

The relevance of having a pseudo-inverse matrix written in terms of the Laplacian matrix eigenvalues and eigenvectors is broad. For example, we can derive analytical results for any generic circulant graph (see Sect. 2.3.2). In this thesis, we are particularly interested in its use for solving the flow problem in conservative networks (see Sect. 3.1.2). Namely, we want to find analytical expressions for the currents that are developed in distribution networks when a set of nodes are identified as constant sources (sinks) of inflow (outflow) and the topology structure of the network is known. In those cases, the problem is formulated mathematically as a Laplacian matrix, which represents the network, times an unknown vector, which represents the loads at each node, equal to the known vector of inflow and outflows at every node of the network. Hence, the problem is solved once the Laplacian matrix of the network is inverted.

In general, there are various situations in this thesis where a solution for a particular problem is found once a Laplacian matrix is inverted. Specifically, whenever we have a vector, $\vec{y} \in \mathbb{R}^N$, of N known elements, y_j, a known matrix $\mathbf{F} \in \mathbb{M}_{N\times N}$, a set of N unknowns x_j, and an equation that relates these three quantities such that

$$y_i = \sum_{j=1}^{N} F_{ij}\,\left(x_i - x_j\right) = \sum_{j=1}^{N} [\mathbf{G}(\mathbf{F})]_{ij}\, x_j, \tag{2.40}$$

where $\mathbf{G}(\mathbf{F})$ is the Laplacian matrix determined by the elements of $\mathbf{F}$ (namely, by $G_{ij} \equiv -F_{ij}$ if $i \neq j$ and $G_{ii} \equiv \sum_{j=1}^{N} F_{ij}$), then, the solution is found inverting the Laplacian matrix $\mathbf{G}(\mathbf{F})$ using Eq. (2.36). Specifically, the operation of the pseudo-inverse Laplacian matrix $\mathbf{X}(\mathbf{F})$, which is defined from the eigenvalues and eigenvectors of $\mathbf{G}(\mathbf{F})$ by Eq. (2.36), on Eq. (2.40) results in

$$\mathbf{X}(\mathbf{F})\,\vec{y} = \mathbf{X}(\mathbf{F})\,\mathbf{G}(\mathbf{F})\,\vec{x} = \left(\mathbf{I} - \frac{1}{N}\mathbf{J}\right)\vec{x} \quad \Rightarrow \quad \vec{x} = \mathbf{X}(\mathbf{F})\,\vec{y} + \langle x\rangle\,\vec{1}, \tag{2.41}$$

where we have used the third property of the pseudo-inverse Laplacian matrix, i.e., Eq. (2.39), and define the average vector, $\langle x\rangle\,\vec{1} \equiv \mathbf{J}\vec{x}/N$ ($\vec{1}$ [$\mathbf{J}$] being the vector [matrix] with entries all equal to 1). In numerous situations, we find in this thesis that the constant term in Eq. (2.41) is cancelled because the physical problems that are being addressed require the difference between the values of the unknowns, namely, $x_i - x_j$, instead of the real magnitudes that Eq. (2.41) provide.

2.3.2 Circulant Networks Spectral Characteristics

The circulant networks constitute a significant part of our derivations for explicit results on the Transmission of Energy and Synchronisation in Complex Networks.

Here, we enunciate their spectral properties, which we define in Sect. 2.1.4. Hence, we focus on the eigenvalues and eigenvectors of the Laplacian matrix $\mathbf{G}$ of the network.

A circulant network holds a circulant matrix representation, namely, its adjacency or Laplacian matrix are circulant. Specifically, a matrix $\mathbf{G} \in \mathbb{M}_{N\times N}$ is called circulant if its entries satisfy $G_{ij} = G_{1,j-i+1}$, where $j-i+1$ is taken as a module N operation. Thus, $\mathbf{G}$ is expressed [21] as

$$\mathbf{G} = \begin{pmatrix} g_1 & g_2 & g_3 & \cdots & g_{N-1} & g_N \\ g_N & g_1 & g_2 & \cdots & g_{N-2} & g_{N-1} \\ g_{N-1} & g_N & g_1 & \cdots & g_{N-3} & g_{N-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ g_2 & g_3 & g_4 & \cdots & g_N & g_1 \end{pmatrix}. \tag{2.42}$$

Because of the matrix form of Eq. (2.42), the circulant network's matrix representations are expressed solely with the first row. Moreover, its Laplacian matrix is symmetric, which implies a real spectra of eigenvalues (Sect. 2.2.3). In particular, the eigenvalues are found from [21]

$$\lambda_n(\mathbf{G}) = g_1 + g_2\,\omega_n + g_3\,\omega_n^2 + \cdots + g_N\,\omega_n^{N-1},\ \forall n = 1,\ \ldots,\ N, \tag{2.43}$$

where $\omega_n \equiv e^{i\,2\pi\,(n-1)/N}$, $i = \sqrt{-1}$ being the imaginary number, and the diagonal element g_1 is given by $g_1 = -\sum_{k=2}^{N} g_k$. Hence, $\lambda_1 = 0$. The rest of the eigenvalues are positive if $g_k \leq 0$ for all $k > 1$. The reason for this last condition is that the Laplacian matrix becomes positive semi-defined if $g_k \leq 0,\ \forall k > 1$ (see Sect. 2.2.4).

In Ref. [21], an explicit expression for the eigenvalues and eigenvectors of circulant Laplacian matrix with positive semi-defined properties is derived. Their result for the eigenvalues is

$$\lambda_n(\mathbf{G}) = \sum_{k=1}^{N} g_k\,\cos\left[\frac{2\pi\,(n-1)}{N}(k-1)\right],\ \forall n = 1,\ \ldots,\ N, \tag{2.44}$$

which is straightforwardly derived from Eq. (2.43) when taking the real part of both sides of the equality. These equality is extremely helpful when dealing with circulant networks and, in particular, to this thesis. Similarly, the explicit expression for the eigenvectors, $\vec{\psi}_n$, coordinate k, is given by

$$\left[\vec{\psi}_n\right]_k = \frac{1}{\sqrt{N}}\left(\cos\left[2\pi\,\frac{(n-1)}{N}(k-1)\right] + \sin\left[2\pi\,\frac{(n-1)}{N}(k-1)\right]\right). \tag{2.45}$$

We note from Eq. (2.45) that any circulant network shares the same eigenvector base since the expression is independent of g_k. Moreover, if the Laplacian matrix of the network is also positive semi-defined (i.e., $g_k < 0\ \forall k > 1$, because $g_1 = -\sum_{k=2}^{N} g_k$), then, Eq. (2.44) provides an explicit way to calculate its eigenvalues.

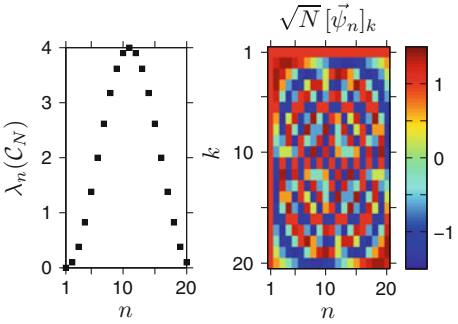

Fig. 2.11 The left (*right*) panel shows the eigenvalues, $\lambda_n(\mathcal{C}_N)$ (eigenvectors, $\vec{\psi}_n$), of the Laplacian matrix of a ring graph, $\mathcal{C}_N$, of $N = 20$ nodes. The colour code in the right panel indicates the value of the kth eigenvector's coordinate without normalisation (i.e., multiplied by $\sqrt{N}\vec{\psi}_n$). Both quantities are derived by their explicit formulas, namely, by Eqs. (2.44) and (2.45)

In particular, the magnitudes of these eigenvalues are the quantity distinguishing the differences between circulant networks with different node degrees.

As a working example, we apply the solution of Eqs. (2.44) and (2.45) to a ring graph, namely, to $\mathcal{C}_N$, with $N = 20$ nodes and unit weights (i.e., $A_{i,i+1} = 1$, $\forall\, i = 1, \ldots, N$ in module N, otherwise $A_{ij} = 0$). The spectral characteristics are shown in Fig. 2.11. Specifically, the set of unordered eigenvalues is given [13] by $\lambda_n = 2 - 2\cos[2\pi\,(n-1)/20]$, which is equal to $\lambda_n = 2 - \cos[2\pi\,(n-1)/20] - \cos[2\pi\,(n-1)\,19/20]$ derived from Eq. (2.44). From the right panel, we note that the eigenvectors are orthogonal as expected because the coordinate values take a certain skew symmetry. Also, all eigenvectors in this right panel have a unit value at the first coordinate, corresponding to the first row in this panel [$k = 1$ in Eq. (2.45)], with the exception of the first column eigenvector, corresponding to the first column in this panel, which is such that $\sqrt{N}\vec{\psi}_1 = \vec{1}$ always.

Circulant networks are extremely useful because of their explicit spectral characteristics. Moreover, these networks can be used for perturbation approaches. In other words, networks that have a strong regular component can be first approximated by a circulant networks and then be corrected using a perturbation approach based on the Eqs. (2.44) and (2.45).

2.3.3 Equivalent Resistance, Its Bounds, and the Kirchhoff Index

The *equivalent resistance* between two nodes i and j of a connected network is [19–23]

$$\Upsilon_{ij} = \sum_{n=2}^{N} \frac{1}{\lambda_n} \left| \left[\vec{\psi}_n\right]_i - \left[\vec{\psi}_n\right]_j \right|^2, \tag{2.46}$$

where $\vec{\psi}_n$ [λ_n] is the kth eigenvector (eigenvalue) of the Laplacian matrix of the network, with $\lambda_1 = 0$. The magnitude of Eq. (2.46) is equal to the one found by Circuit Theory [24] or by Green functions [18] in symmetric resistor networks.

The definition of equivalent resistance given by Eq. (2.46) is directly related to the pseudo-inverse Laplacian matrix, also known as Moore-Penrose inverse matrix, $\mathbf{X}$, which we define in Eq. (2.36) in Sect. 2.3.1. Using $\mathbf{X}$ and the expansion of Eq. (2.46), the equivalent resistance is given in terms of $\mathbf{X}$ entries by [19–23]

$$\Upsilon_{ij} = X_{ii} + X_{jj} - X_{ij} - X_{ji}. \tag{2.47}$$

which for an symmetric network results in $\Upsilon_{ij} = X_{ii} + X_{jj} - 2X_{ij}$.

In Circuit Theory, the equivalent resistance between two points i and j of a circuit that is connected by a series of resistors, $\{R_{ik}, \ldots, R_{lj}\}$, is determined from

$$R^{(eq)} = R_{ik} + \cdots + R_{lj}. \tag{2.48}$$

On the other hand, if the two points are connected by L parallel resistors, $\{R_{ik}^{(1)}, \ldots, R_{lj}^{(L)}\}$, then, the equivalent resistance is determined from

$$\frac{1}{R^{(eq)}} = \frac{1}{R_{ij}^{(1)}} + \cdots + \frac{1}{R_{ij}^{(L)}}. \tag{2.49}$$

These two equations are straightforward to calculate when the circuit is a regular resistor network. In other words, Eqs. (2.48) and (2.49) are useful when the topology of the connections is simple enough to be able to differentiate the paths connecting two nodes into series and parallel paths. However, when the topology is complex, as in most real-world networks, then, the equivalent resistance is better computed from Eq. (2.46). Hence, for complex networks, the equivalent resistance between any two nodes requires the Laplacian matrix representation (including the edge weights, which are the resistors in the circuit networks) and its eigenvalues and eigenvectors.

In particular, we note that Eqs. (2.48) and (2.49) have an extended version that is valid for circuit networks that contain capacitive and inductive elements in their edges. Namely, the resistance values turn into impedance values and the ER is an equivalent impedance value. These equivalence is maintained when dealing with steady-state currents, a topic which corresponds to the starting point of our transmission of Energy problem and results (details are given in Sect. 3.1).

From the definition [Eq. (2.46)] of the equivalent resistance between two nodes of a network and its Circuit Theory analogy, we note that the value of Υ_{ij} is a representation of the amount and type of paths connecting nodes i and j. Hence, it is a topological metric for the network that contains more information than the number of paths between the nodes or the topological distance. Its value tells us how hard it is to get from node i to j, using the fact that parallel paths are an optimal option (less energy consumption) and series paths are a detrimental option (more energy

consumption). Moreover, because it takes into account all the paths connecting the two nodes, it is also useful to diminish the complexity of the topology.

An strict upper bound for Υ_{ij} is found by expanding Eq. (2.46). Assuming a symmetric network structure, the quantities in Eq. (2.46) are real, hence, the expansion holds

$$\Upsilon_{ij} = \sum_{n=2}^{N} \left(\frac{\left[\vec{\psi}_n\right]_i^2}{\lambda_n} + \frac{\left[\vec{\psi}_n\right]_j^2}{\lambda_n} - 2\frac{\left[\vec{\psi}_n\right]_i \left[\vec{\psi}_n\right]_j}{\lambda_n} \right) < 2(1-\delta_{ij}) \sum_{n=2}^{N} \frac{1}{\lambda_n}, \quad (2.50)$$

which is the result of observing that $[\vec{\psi}_n]_i^2 < 1$ due to the normalisation of the eigenvectors. Moreover, a similar upper bound is also found if all pairs of nodes are considered. Namely, $\sum_{i=1}^{N}\sum_{j=1}^{N} \Upsilon_{ij} = 2N \sum_{n=2}^{N} 1/\lambda_n$.

The *Kirchhoff index*, $Kf(\mathcal{G})$, of a network, $\mathcal{G}$, is an invariant quantity that is defined by the sum of the inverse of the non-null eigenvalues of its Laplacian matrix $\mathbf{G}$ [3]. Specifically,

$$Kf(\mathbf{G}) \equiv N \sum_{n=2}^{N} \frac{1}{\lambda_n(\mathcal{G})}. \quad (2.51)$$

Consequently, the upper bound for the equivalent resistance from Eq. (2.50) depends on the Kirchhoff index of the graph. As an invariant quantity, Kf is also useful to characterise different network topologies.

Another upper bound, smaller than the upper bound derived in Eq. (2.50), is found assuming that $\lambda_n \simeq \lambda_2$ for all eigenmodes, hence,

$$\Upsilon_{ij} \leq \frac{1}{\lambda_2} \sum_{n=2}^{N} \left| \left[\vec{\psi}_n\right]_i - \left[\vec{\psi}_n\right]_j \right|^2 = 2\frac{(1-\delta_{ij})}{\lambda_2}, \quad (2.52)$$

where the last equality is found from using the orthogonal properties of the eigenvectors, namely, using that $\sum_{n=1}^{N} [\vec{\psi}_n]_i [\vec{\psi}_n]_j = 1/N + \sum_{n=2}^{N} [\vec{\psi}_n]_i [\vec{\psi}_n]_j = \delta_{ij}$. Similarly, assuming that $\lambda_n \simeq \lambda_N$ for all eigenmodes, a lower bound is found for the equivalent resistance. That is,

$$\Upsilon_{ij} \geq \frac{1}{\lambda_N} \sum_{n=2}^{N} \left| \left[\vec{\psi}_n\right]_i - \left[\vec{\psi}_n\right]_j \right|^2 = 2\frac{(1-\delta_{ij})}{\lambda_N}. \quad (2.53)$$

The bounds in Eqs. (2.52) and (2.53) are relevant for bounding the edge capacities we derive for steady-state flow networks in Sect. 3.1.5.

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