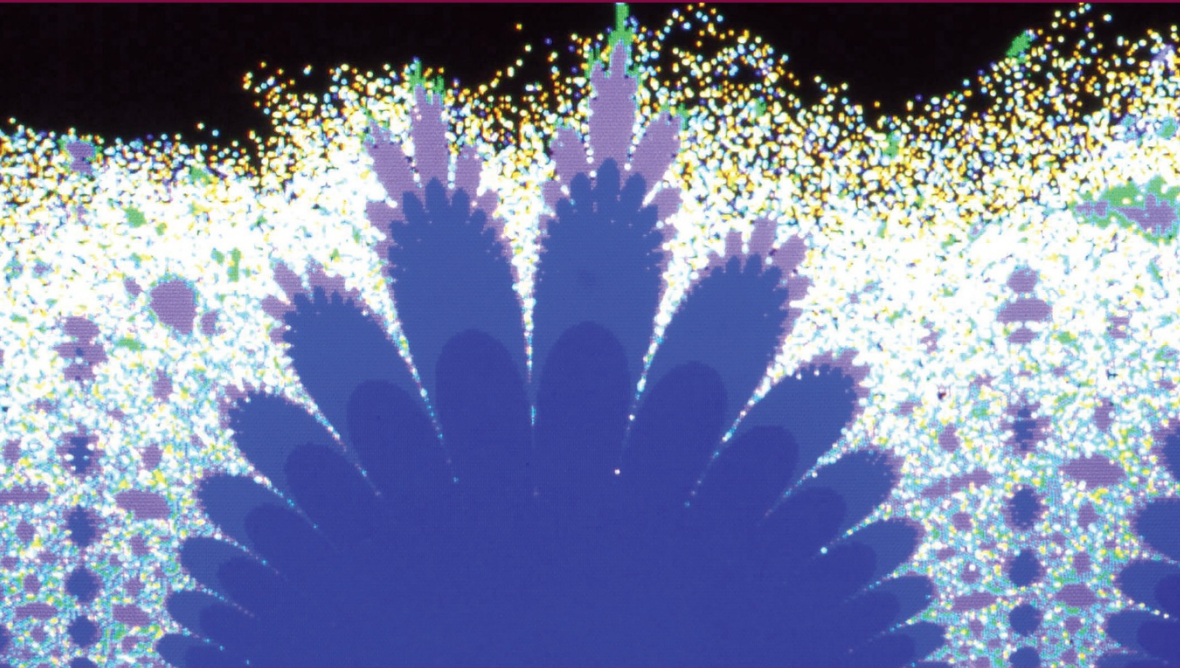


MECHANICAL ENGINEERING AND SOLID MECHANICS SERIES



# Fractional Dynamics on Networks and Lattices

**Thomas Michelitsch**  
**Alejandro Pérez Riascos**  
**Bernard Collet**  
**Andrzej Nowakowski**  
**Franck Nicolleau**



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## Fractional Dynamics on Networks and Lattices



*Series Editor*  
*Noël Challamel*

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## Preface

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Random walks are among the most fundamental stochastic processes that occur ubiquitously in various interdisciplinary contexts such as in biological networks, the foraging of animals, the spread of diseases, in finance, human mobility in cities, friendship networks, among many other “complex systems”. Generally, random walks are microscopic models for diffusion processes and play a crucial role in the development of “random search” strategies. One of the main goals of this field is to find a strategy that a given set of targets distributed among a larger set is most quickly visited by the walker. This and similar questions constitute one of the major motivations and driving forces for the subjects of this book. The analysis of new random walk strategies, especially those which allow faster exploration of a network or a subset of it, is highly desirable for many interdisciplinary applications and interesting from a theoretical point of view. Last but not least, the recent upswing of online networks such as Google and social networks has launched a huge interest in stochastic motions on networks. In many of these problems of real life such as in population dynamics, chaotic motions, the time evolution of stock-market prices and many others, it is impossible and even meaningless to describe time evolutions using deterministic equations. Instead, one is interested in extracting a maximum of “statistical information” from these processes. As a result, many different kinds of random walk models have been proposed and extensively studied.

The “random walk history” started more than a century ago when the notion of “random walk” was coined by K. Pearson in 1905 coming along with the groundbreaking works of A. Einstein who formulated the stochastic motion of particles, and similar ideas were developed by M. von Smoluchovski at about the same time. Then later on P. Lévy together with R. von Mises, A. Kolmogorov, N. Wiener, L. Doob and K. Itô were among the founders of modern probability theory, and many further classical works are connected with the names of L. Bachelier, R. Brown, G. Pólya, Lord Rayleigh, W. Feller, M. Kac, F. Spitzer, A. Khinchin, E.W. Montroll, G.H. Weiss, A.A. Markov, B. Mandelbrot and many

others. The systematic study of random walks was probably inspired by the “Gambler’s Ruin” problem, which was analyzed by Bernoulli, Fermat, Huygens, Pascal, among others.

Random walks are today a highly interdisciplinary basic approach to statistical physics. In the meantime, a burst of remarkable literature has been published on the subject. The features of random motions depend sensitively on the topology of the “environments” and “spaces” where they occur. Many of them can be conceived as taking place on well-defined and countable sets of “states”. If these sets of states are finite and countable, then they can be considered as (finite) graphs or synonymously networks. When random transitions within these well-defined sets of states occur, then we can describe these processes as “random walks on graphs”. In more general situations, where random walks are performed either in continuous compact spaces or on disjoint (often fractal sub-) sets where the points are uncountable, it appears to be fruitful to describe such walks in terms of “probability measures” by means of the language of measure theory.

G. Pólya was one of the first to demonstrate the importance to study random walks on simple multidimensional integer lattices. He disclosed in a celebrated paper the crucial role of the dimension of the lattice for the recurrence/transience behavior of a walk. This behavior emerges in the so-called Pólya walks having a most simple generating law, namely, that the walker in one time step can jump with equal probabilities only to connected neighbor nodes. The great achievement of that work was also to have shown that universal behavior can be obtained already by most simple generating laws. We consider in Chapter 7 a generalization of the Pólya walk problem and by assuming a “fractional generating law” we derive a generalized recurrence theorem as a universal feature of the “fractional random walk” and all walks with asymptotic Lévy flight behavior emerging from the fractional dynamics on infinite multidimensional lattices and spaces.

We will see in the course of this book that whatever be the generating law for a Markovian walk on an undirected network, after sufficiently many time steps the probability distributions may converge only to two distinct kinds of limiting distributions, namely either Gaussian distributions when the jump lengths on the network in one time step are limited (e.g. to neighbor nodes or light-tailed distributed to further distant neighbors) with *finite mean squared jump distance*, or Lévy distributions when the jump lengths on the network are heavy tailed with *infinite mean square jump distance*. Any further complication or sophistication in the generating laws apart from these essential features does not affect this universal asymptotic behavior. We will analyze these behaviors for Markovian walks on networks thoroughly in the course of the book. By this observation for the behavior after sufficiently long times of observation, it is sufficient to consider “simple” generating laws leading to the same of the two possible *universal asymptotic behaviors* as the “real” perhaps complicated unknown generating law.

In this book, we uniquely consider Markovian walks where the walker undertakes uncorrelated steps on a network or in the continuum limit on a continuous space. We mainly analyze time discrete walks but also derive limiting transitions to time continuous walks. One principal focus is concentrated on the analysis of “long-range navigation” of walks with “long-range steps” where the walker in one-time step can reach far distant nodes. The notion of “distance” may appear in two different senses, either as the distance on the network counting the smallest number of steps between two nodes, or especially important for continuum limit analysis, where “distance” means the Euclidean distance in the embedding space. “Long-range step” means in the first place that the walker during one-time step can cover a large “network distance”.

For different kinds of random walks, especially walks exhibiting long-distance jumps strategies, we derive dynamic characteristics such as first passage quantities, mean occupation times, the number of distinct nodes visited by a walker, recurrence features and several further quantities of interest. One might expect that there is an infinite family of generating laws leading to an infinite set of different long-range behaviors. However, as mentioned on “sufficiently large” networks the limiting distributions after sufficiently large observation times (on undirected connected networks and lattices) are either Gaussian distributions with Brownian motion or Lévy distributions with Lévy flights. Both cases can be classified by symmetric  $\alpha$  stable distributions where the only real long-range navigation that is stable toward rescaling of the network are “fractional walks” with fat-tailed (Lévy) distributions emerging after many time steps. The jump patterns that occur from such heavy-tailed jump distributions with the occurrence of long-range steps leading to diverging mean square jump distances are indeed characteristic for Lévy flights (these can also be referred to as Lévy motions). This behavior is contrasted by the finite mean square displacements of normal diffusive Brownian motions with localized short-distance jumps.

The present book consists of two parts comprising eight principal chapters. The first part “Dynamics on General Networks” (Chapters 1–5) is devoted to the analysis of Markovian random walk features that generally hold in *connected undirected networks* where we consider both finite and infinite networks. The second part “Dynamics on Lattices” (Chapters 6–8) is devoted to Markovian walks that take place on regular networks and lattices such as hyper-tori and multidimensional integer lattices. All results presented and discussed are systematically derived either within the main text in the chapters or, when the derivations become too lengthy or may disturb the course of the explanations, we have put them into appendices at the ends of the chapters. In the derivations, we have chosen a rather intuitive approach avoiding a formalistic and abstract level of the proofs. All the derivations are performed by employing elementary mathematical methods that students of physics, engineering science or mathematical disciplines in a progressed level should be familiar with.

In Chapter 1, we give a general introduction to basic graph theory where we introduce the *Laplacian matrix* containing the topological information of the network. We also consider some examples such as the ring and interacting cycles where the eigenvectors and eigenvalues of the Laplacian matrix are explicitly known. In this chapter, we derive the good properties of Laplacian matrices and define matricial functions of the Laplacian matrix that conserve these good properties. In this way, we can later define generalized random walk strategies with new generating rules allowing fast navigation and long-range moves on the network. Among the most interesting candidates, we identified power law matrix functions of the Laplacian matrix, the so-called “*fractional Laplacian matrix*”, where we demonstrate in detail that its powers are restricted to be between zero and one. We will see in the course of the book that the fractional Laplacian stands out to be the essential generator for asymptotically scale-free long-range navigation and emergence of Lévy flights. Once we have derived the good properties that admissible Laplacian matrix functions need to fulfill, we construct these functions and obtain, when these functions are continuously differentiable, the family of good Laplacian functions as a class of functions with completely monotonic derivatives. In all cases, the family of good Laplacian functions constitutes a certain class of “Bernstein functions”. An essential outcome of this chapter is that any admissible Laplacian matrix function starts with the lowest order either with the Laplacian matrix (“type (i) matrix functions”) or by non-integer fractional power of the Laplacian matrix where the power is restricted between zero and one (“type (ii) matrix function”). Then, we consider several examples of admissible Laplacian matrix functions that define new random walk strategies. We demonstrate in the course of the book, coming from several directions, that the lowest order determines the limiting distribution of the walks generated by these functions after many time steps, namely type (i) walks converge to Gaussian distributions and type (ii) walks to Lévy distributions given that the network is sufficiently large. This universal limiting behavior is purely determined by the lowest orders of the series expansion of the functions explored. The effect of all the higher orders is wiped out and therefore is irrelevant.

In Chapter 2, we discuss a particular case of the Laplacian functions that maintain the good structure of the Laplacian as outlined in Chapter 1 to explore the properties of the fractional Laplacian of a network. The introduction of the fractional Laplacian is motivated by the emergence of long-range correlations in a network. In this way, by using this information we can define different global quantities and dynamical processes that consider the whole structure of a network. We discuss the construction of Laplacian matrix functions and obtain integral representations, especially for the fractional Laplacian matrix by Mellin transforms being equivalent to the so-called “*Lévy-Kintchin representation*” by employing Lévy densities or Lévy measures. In the appendix of Chapter 2 (section 2.5) we briefly discuss some basic relations and definitions of “measures” by considering “*probability measures*”.

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In Chapter 3, we analyze general properties of Markovian random walks on finite connected (undirected) networks where we can identify this type of walk with *Markov chains*. The generating laws of time-discrete Markovian random walks are defined by master equations involving the (one-step) transition matrix that contains the Laplacian matrix (function) of the walk. We deduce good properties for a Markovian random walk on connected finite graphs and relate these good properties to *ergodicity* and *aperiodic ergodicity* of the Markov chain. We perform a detailed analysis of the spectral properties of ergodic (irreducible) and aperiodic ergodic Markov chains and consider some basic laws such as the “*fundamental theorem of Markov chains*” and ergodic hypothesis and theorem of Markov chains. We further discuss the relation to the “*strong law of large numbers*”. We derive further the stationary distribution of normal walks (walks simply generated by the Laplacian matrix) allowing only steps to connected neighbor nodes, and we obtain in this way the mean recurrence time for finite Markov chains (Kac’s formula). Also, we discuss in this chapter periodic ergodicity as realized in bipartite graphs and analyze the related spectral structure of the one-step transition matrix. In an appendix, we analyze the asymptotic behavior of the transition matrix of classical Pólya walks taking place on infinite multidimensional integer lattices  $\mathbb{Z}^d$  that are bipartite. We show there that in such classical Pólya walks Gaussian distributions emerge after many time steps.

In Chapter 4, we explore the good properties of a Laplacian matrix to obtain a Markovian stochastic random walk (one-step) transition matrix defining the transition probabilities between the nodes of a network in order to generalize random walk strategies to obtain walks with long-distance steps. The chapter is devoted to a systematic study of the non-local dynamics generated by a series of important good Laplacian matrix functions where we investigate characteristics describing the speed of the navigation on the network such as global times the walker needs to visit any node of the network. In this study, the outstanding random walk search capacity of the “fractional walk” is demonstrated.

In Chapter 5, we discuss fractional classical versus fractional quantum transport. First, in this chapter, by starting with master equations defining the random walks on multidimensional lattices, we derive two cases. (1) The classical normal diffusion equation as a continuum limit of a “normal walk” where the step length is constant. This case corresponds to a Pólya type walk on the lattice. (2) The fractional diffusion equation obtained from a master equation with inverse power law fat-tailed step distributions. This walk corresponds to a “fractional walk” (Lévy flight) on the lattice. After deducing several key quantities, such as return probabilities to the departure nodes for the classical walk, we discuss the fractional Schrödinger equation and its network counterpart. In this way, we analyze several essential universal features of fractional quantum walks where remarkable phase effects generate universal behavior independent from the fractional index that characterizes the search efficiency of the fractional quantum walk.

The second part of the book, “Dynamics on Lattices”, is devoted to the analysis of Markovian walks in lattices where we strongly focus on the “fractional random walk” generated by fractional powers of the Laplacian matrix. In Chapter 6, we consider as the most simple one-dimensional cases finite and infinite rings. First, we derive an explicit form of the *fractional Laplacian matrix* for the *infinite* ring and use this result to construct the fractional Laplacian matrix for the *finite* ring. Finally, we deduce pertinent continuum limit distributions of nodes: the infinite space continuum limit and the periodic string continuum limit. In these continuum limits, the fractional Laplacian matrix takes the distributional representations of the kernels of the fractional Laplacian kernel (Riesz fractional derivative kernel). These explicit representations allow a thorough explicit analysis of the fractional walk and its continuum limits on rings. In this chapter, uniquely the fractional operators that generate the fractional walk on the ring and their continuum limits are derived. These results are then employed for an explicit analysis of the fractional walk on the infinite ring in Chapter 7.

In Chapter 7, we consider the fractional walk, i.e. the Markovian random walk that is generated by the fractional power of the Laplacian matrix on the  $d$ -dimensional ( $d = 1, 2, 3, 4, \dots$ ) periodic  $d$ -torus and the infinite lattice limit, which is the  $d$ -dimensional integer lattice  $\mathbb{Z}^d$ . We introduce basic quantities characterizing random walks such as the probabilities of *first passage*; the numbers of first passage paths connecting a pair of nodes; the probability that a node is *ever* visited; the mean first passage time (MFPT), i.e. the number of time steps the walker is expected to need to visit a node; the *mean occupation time* or mean residence time (MRT) the walker stays on a node or a set of nodes; the mean recurrence time (Kac formula); the mean step distance (MSD) (or average velocity) of the walker and the number of distinct nodes visited by the walker, among other characteristics. We analyze these characteristics for the “fractional random walk”, i. e. the random walk generated by a fractional non-integer power of the Laplacian matrix (with an admissible exponent between zero and one). This walk is the “fractional” generalization of the classical Pólya walk. We derive in this chapter the recurrence theorem for this walk (being the fractional counterpart of Pólya’s recurrence theorem) where the fractional walk for exponent one recovers the Pólya walk and Pólya’s recurrence theorem. We further derive asymptotic representations for the Green’s function matrix for the fractional walk where its symmetric elements have the interpretation of mean occupation times. In the recurrent regime, the Green’s function diverges due to infinitely many returns to nodes, whereas in the transient regime the Green’s function exists and is finite. We derive for the transient regime the asymptotic representation of the Green’s function (far from the departure node) taking the representation of Riesz potentials where in the Pólya limit the classical Newtonian potentials are recovered. In the second part, the fractional walk on the infinite ring is analyzed. For the infinite ring, all results including the Green’s functions and their Riesz limits are derived in an explicit form by utilizing the results of Chapter 6.



Finally, Chapter 8 is devoted to the asymptotic analysis of Markovian walks on undirected networks. We derive from the characteristic matrices such as the Laplacian matrix, adjacency matrix and transition matrix continuum limit kernels, which have to be conceived as distributions or generalized functions. Further, we deduce the convolutional diffusion equation governing the asymptotic behavior of Markovian walks. We especially focus on universal asymptotic behavior, i.e. the limiting probability distributions that emerge after sufficiently many time steps in the infinite network limits. We further introduce some “constitutive assumptions” on the node distributions in the infinite multidimensional embedding space where we assume spatially homogeneous and isotropic node distributions leading to isotropic kernels. We analyze especially the distinct asymptotic behavior of types (i) and (ii) Laplacian kernels, where type (i) corresponds to light-tailed adjacency density kernels and type (ii) corresponds to heavy-tailed adjacency density kernels. We deduce the limiting distributions of walks generated by types (i) and (ii) densities: the probability density functions (PDFs) of type (i) walks converge to Gaussian distributions, whereas the PDFs of type (ii) walks converge to Lévy distributions. As an example, we consider the Pearson walk that serves as a proto-example for a type (i) walk with restricted (constant) step distance that the walker can cover in one-time step. We also derive for the transient regime the asymptotic Riesz potential Green’s functions for type (ii) walks taking in the Pólya walk limit (representing hence the universal asymptotic Green’s functions of all type (i) walks) the representations of Newtonian potentials. In this way, we demonstrate again the emergence of Brownian motions for type (i) walks where the steps lengths are drawn from normal distributions, and for type (ii) walks the asymptotic emergence of Lévy flights where the step lengths are drawn from Lévy distributions. At the end of this chapter, we outline some ideas about how to approach the asymptotic behavior of fractal node distribution by considering a Cantor dust distribution of nodes. In the appendices of this chapter, we derive several important integrals and normalization constants that occur repeatedly in the context of Lévy flights and the involved fractional continuum limit distributional kernels. Especially we outline some properties of  $\alpha$ -stable symmetric distributions occurring as limiting PDFs in the present analysis. We also derive the “spectral dimension” of Lévy flights in an appendix (section 8.4). The spectral dimension is a generalization of the dimension of the reciprocal (dual) state space. In all demonstrations, we try to give physical interpretations to the derived quantities, and special care is taken with signs of the kernels and their physical interpretations related to the stochastic properties of PDFs.

The present book represents a snapshot of some of our present results and is an attempt to relate them with state-of-the-art contexts. At the same time, we hope that this attempt may bear some fruit in terms of inspiration for the reader. We are happy to receive any feedback.

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January 2019

PART 1

# Dynamics on General Networks



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# Characterization of Networks: the Laplacian Matrix and its Functions

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## 1.1. Introduction

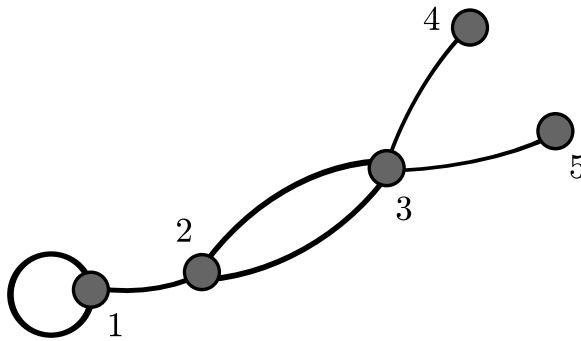
The study of networks, their characteristics and dynamical processes taking place on these structures have had a significant impact in different fields of science and engineering, leading to important applications in the context of physics, biology and social and computer systems among many others. In 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  $i = 1, 2, \dots, N$  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

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

where  $\{v_i\}_{i=0}^n \subseteq \mathcal{V}$ ,  $\{e_i\}_{i=1}^n \subseteq \mathcal{E}$ . For  $j = 1, \dots, n$ , 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  $\mathcal{W} = (v_0, v_1, \dots, v_n)$ , 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  $i, j = 1, 2, \dots, N$ , where  $\delta_{ij}$  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

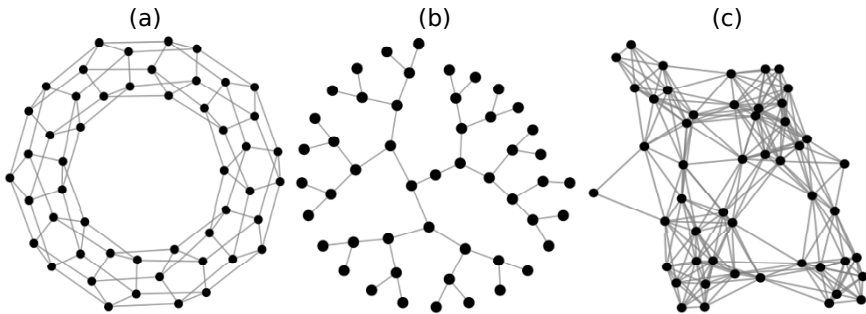
In the following, we use the term *network* to denote simple connected graphs; in addition, variations of this term are common. For example, in directed networks we include information about the direction of the edges; on the other hand, the term weighted network refers to networks with additional information 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

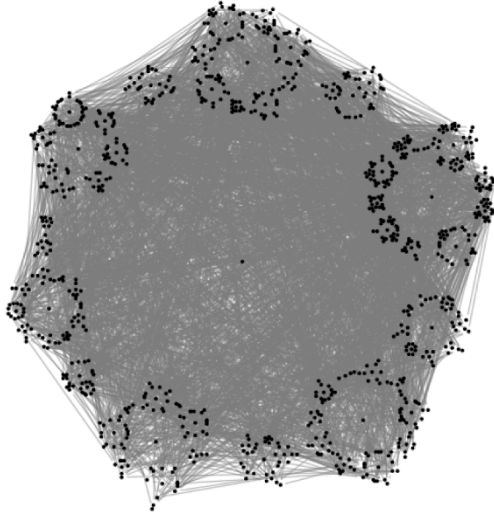
Other large-world networks are found in the study of fractal networks that arise by implementing various algorithms that can be deterministic or random. In the context of real networks, we find large-world networks in the analysis of transport networks like streets, subway stations, electric towers networks [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 Erdős–Rényi (1959), Watts–Strogatz (1998) and Barabási–Albert (1999).

In the Erdős–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.** Erdős–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

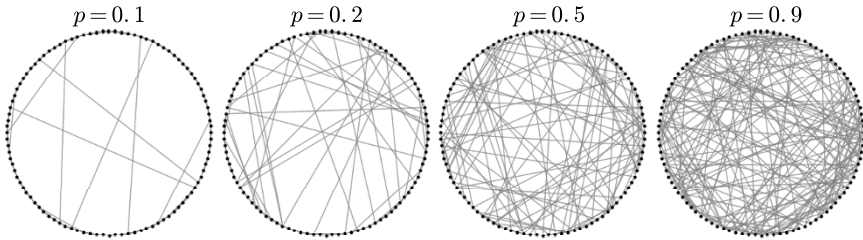
For an Erdős–Rényi network, the average value of the number of lines in  $\mathcal{G}_{N,p}$  is  $pN(N-1)/2$  and the average degree is  $\langle k \rangle = p(N-1)$ . On the other hand, the probability  $P(k)$  to obtain a node with degree  $k$  is given by [BOL 01, BAR 08b]:

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

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  $N \rightarrow \infty$ , 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 Erdős–Rényi model is named after Paul Erdős, 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 Erdős–Rényi random network. In Figure 1.4, we represent different cases of Watts–Strogatz networks with  $N = 20$  nodes obtained for different rewiring probabilities  $p$ .

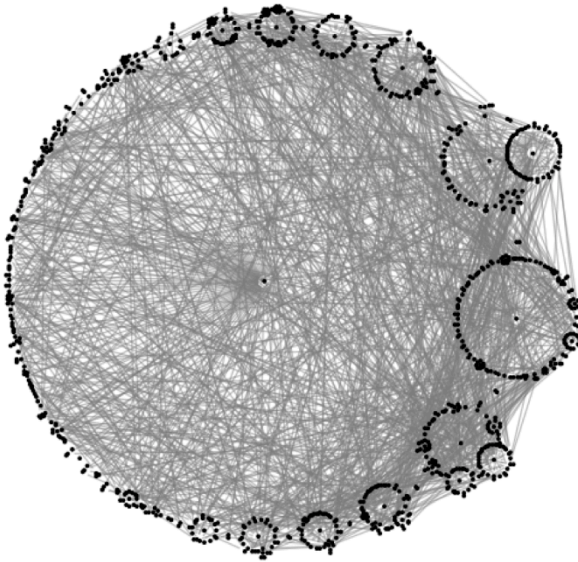


**Figure 1.4.** *Watts–Strogatz model. In this example, the initial network is a ring with  $N = 20$  nodes. We add lines to connect each node to its two next neighbor's neighbor nodes, and the resulting structure has a constant degree  $k = 4$ . Then, for  $0 < p < 1$  edges are randomly selected and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

$$L_{ij} = k_i \delta_{ij} - A_{ij} \quad [1.2]$$

for  $i, j = 1, 2, \dots, N$ , where  $\delta_{ij}$  denotes the Kronecker delta. In matricial 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]

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

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

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

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

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

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

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

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

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

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].