1
Introduction

Despite the fact that complex networks are the driving force behind the investigation of the spectra of graphs, it is not the purpose of this book to dwell on complex networks. A generally accepted, all-encompassing definition of a complex network does not seem to be available. Instead, complex networks are understood by instantiation: the Internet, transportation (car, train, airplane) and infrastructural (electricity, gas, water, sewer) networks, biological molecules, the human brain network, social networks, software dependency networks, are examples of complex networks. By now, there is such a large literature about complex networks, predominantly in the physics community, that providing a detailed survey is a daunting task. We content ourselves here with referring to some review articles by Strogatz (2001); Newman *et al.* (2001); Albert and Barabasi (2002); Newman (2003b), and to books in the field by Watts (1999); Barabasi (2002); Dorogovtsev and Mendes (2003); Barrat *et al.* (2008); Dehmer and Emmert-Streib (2009); Newman (2010), and to references in these works. Application of spectral graph theory to chemistry and physics are found in Cvetković *et al.* (1995, Chapter 8).

Complex networks can be represented by a graph, denoted by G, consisting of a set $\mathcal{N}$ of N nodes connected by a set $\mathcal{L}$ of L links. Sometimes, nodes and links are called vertices and edges, respectively, and are correspondingly denoted by the set V and E. Here and in my book on *Performance Analysis* (Van Mieghem, 2006b), a graph is denoted by $G(\mathcal{N}, \mathcal{L})$ or $G(N, L)$ to avoid conflicts with the expectation operator E in probability theory. There is no universal notation of a graph, although in graph theory $G = (V, E)$ often occurs, while in network theory and other applied fields, nodes and links are used and the notation $G(N, L)$ appears. None of these notations is ideal nor optimized, but fortunately in most cases, the notation G for a graph seems sufficient.

Graphs, in turn, can be represented by a matrix (**art.** 1). The simplest among these graph-associated matrices is the adjacency matrix A, whose entries or elements are

$$a_{ij} = 1_{\{\text{node } i \text{ is connected to node } j\}} \tag{1.1}$$

where 1_x is the indicator function and equal to one if the x is true, else it is zero.

All elements a_{ij} of the adjacency matrix are thus either 1 or 0 and A is symmetric for undirected graphs. Unless mentioned otherwise, we assume in this book that the graph is undirected and that A (and other graph-associated matrices) are symmetric. If the graph consists of N nodes and L links, then **art.** 151 demonstrates that the $N \times N$ symmetric adjacency matrix can be written as

$$A = X \Lambda X^T \tag{1.2}$$

where the $N \times N$ orthogonal matrix X contains as columns the eigenvectors $x_1, x_2, ..., x_N$ of A belonging to the real eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$ and where the matrix $\Lambda = \text{diag}(\lambda_k)$. This basic relation (1.2) equates the topology domain, represented by the adjacency matrix, to the spectral domain of the graph, represented by the eigensystem in terms of the orthogonal matrix X of eigenvectors and the diagonal matrix Λ with corresponding eigenvalues. The major difficulty lies in the map from topology to spectral domain, $A \rightarrow X \Lambda X^T$, because the inverse map from spectral to topology domain, $X \Lambda X^T \rightarrow A$, consists of straightforward matrix multiplications. Thus, most of the efforts in this book lie in computing or deducing properties of X and Λ, given A. Even more confining, most energy is devoted to Λ and the distribution and properties of the eigenvalues $\{\lambda_j\}_{1 \leq j \leq N}$ of A and of other graph related matrices. It is fair to say that not too much is known about the eigenvectors and the distribution and properties of eigenvector components. A state of the current art is presented by Cvetković *et al.* (1997).

1.1 Interpretation and contemplation

One of the most studied eigenvalue problems is the stationary Schrödinger equation in quantum mechanics (see, e.g., Cohen-Tannoudji *et al.* (1977)),

$$H \varphi(r) = E \varphi(r)$$

where $\varphi(r)$ is the wave function, E is the energy eigenvalue of the Hamiltonian (linear) differential operator

$$H = -\frac{\hbar^2}{2m} \Delta + V(r)$$

in which the Laplacian operator is $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, $\hbar = \frac{h}{2\pi}$ and $h \simeq 6.62 \times 10^{-34}$Js is Planck's constant, m is the mass of an object subject to a potential field $V(r)$ and r is a three-dimensional location vector. The wave function $\varphi(r)$ is generally complex, but $|\varphi(r)|^2$ represents the density function of the probability that the object is found at position r. The mathematical theory of second-order linear differential operators is treated, for instance, by Titchmarsh (1962, 1958).

While the interpretation of the eigenfunction $\varphi(r)$ of the Hamiltonian H, the continuous counterpart of an eigenvector with discrete components, and its corresponding energy eigenvalue E is well understood, the meaning of an eigenvector of a graph is rather vague and not satisfactory. An attempt is as follows. The basic

equation (8.1) of the eigenvalue problem, $Ax = \lambda x$, combined with the zero-one nature of the adjacency matrix A, states that the j-th component of the eigenvector x_k belonging to eigenvalue λ_k can be written as

$$\lambda_k (x_k)_j = (Ax_k)_j = \sum_{l=1}^{N} a_{jl} (x_k)_l = \sum_{l \text{ is a direct neighbor of } j} (x_k)_l \qquad (1.3)$$

Since $a_{jj} = 0$, the eigenvector component $(x_k)_j$ weighted (multiplied) by the eigenvalue λ_k equals the sum of the other eigenvector components $(x_k)_l$ over all direct neighbors l of node j. Since all eigenvectors are orthogonal[1], each eigenvector can be interpreted as describing a different inherent property of the graph. What that property means is yet unclear, but the eigenvalue basic equation (1.2) says that there are only N such inherent properties, and the orthogonality of X or of the eigenvectors tells us that these inherent properties are independent. The above component equation (1.3) then expresses that the value $(x_k)_j$ of the inherent property k, belonging to the eigenvalue λ_k and specified by the eigenvector x_k, at each node j equals a weighted sum of those values $(x_k)_l$ over all its direct neighbors l, and each such sum has a same weight λ_k^{-1} (provided $\lambda_k \neq 0$, else one may say that the average over all direct neighbors of those values $(x_k)_l$ is zero). Since both sides of the basic equation (8.1), $Ax = \lambda x$, can be multiplied by some non-zero number or quantity, we may interpret that the value of property k is expressed in different "physical" units. Perhaps, depending on the nature of the complex network, some of these units can be determined or discovered, but the pure mathematical description (8.1) of the eigenvalue problem does not contain this information. Although the focus here is on eigenvectors, equation (1.3) also provides interesting information about the eigenvalues, for which we refer to **art.** 172.

Equation (1.3) reflects a *local* property with value $(x_k)_j$ that only depends the corresponding values $(x_k)_l$ of direct neighbors. But this local property for node j holds *globally* for any node j, with a same strength or factor λ_k. This local and global aspect of the eigenstructure is another fascinating observation, that is conserved after "self-replication". Indeed, using (1.3) with index $j = l$ into (1.3) yields

$$\begin{aligned} \lambda_k^2 (x_k)_j &= \sum_{l_1=1}^{N} a_{jl_1} \sum_{l_2=1}^{N} a_{l_1 l_2} (x_k)_{l_2} = \sum_{l_2=1}^{N} \left(A^2\right)_{jl_2} (x_k)_{l_2} \\ &= d_j (x_k)_j + \sum_{l_2 \text{ is a second hop neighbor of } j} (x_k)_{l_2} \end{aligned}$$

since (see **art.** 30) $\left(A^2\right)_{jj} = \sum_{k=1}^{N} a_{jk} a_{kj} = \sum_{k=1}^{N} a_{jk}^2$ by symmetry $\left(A = A^T\right)$, and $\sum_{k=1}^{N} a_{jk}^2 = \sum_{k=1}^{N} a_{jk} = d_j$ due to the zero-one nature of a_{ij}, and where d_j is the degree, the number of neighbors, of node j. The idea can be continued and a

[1] Mathematically, the eigenvectors form an orthogonal basis that spans the entire N-dimensional space. Each eigenvector "adds" or specifies one dimension or one axis (orthogonal to all others) in that N-dimensional coordinate frame.

subsequent substitution of (1.3) leads to an expression that involves a sum over all three hops nodes away from node j. Subsequent iterations relate the expansion of the graph around node j in the number of hops m, further elaborated in **art.** 17 and **art.** 36, to the eigenvalue structure as

$$\left\{\lambda_k^m - (A^m)_{jj}\right\}(x_k)_j = \sum_{l_m \text{ is an } m\text{-th hop neighbor of } j} (x_k)_{l_m} \tag{1.4}$$

Again, this local expansion around node j holds globally for any node j.

The alternative representation (8.31)

$$A = \sum_{k=1}^{N} \lambda_k x_k x_k^T$$

shows that there is a hierarchy in importance of the properties, specified by the absolute value of the eigenvalues, because all eigenvectors are scaled to have equal unit norm. In particular, possible zero eigenvalues contain properties that the graph does not possess, because the corresponding eigenvectors do not contribute to the structure – the adjacency matrix A – of the graph. In contrast, the properties belonging to the largest (in absolute value) eigenvalues have a definite and strong influence on the graph structure.

Another observation[2] is that the definition of the adjacency matrix A is somewhat arbitrary. Indeed, we may agree to assign the value α to the existence of a link and β otherwise, where α and $\beta \neq \alpha$ can be any complex number. Clearly, the graph is then equally well described by a new adjacency matrix $A(\alpha, \beta) = (\alpha - \beta) A + \beta J$, where J is the all-one matrix. Unless $\alpha = 1$ and $\beta = 0$, the eigenvalues and eigenvectors of $A(\alpha, \beta)$ are different from those of A. This implies that an entirely different, but still consistent theory of the spectra of graphs can be built. We have not pursued this track here, although we believe that for certain problems a more appropriate choice of α and β may simplify the solution.

When encountering the subject for the first time, one may be wondering where all the energy is spent, because the problem of finding the eigenvalues of A, reviewed in Chapter 8, basically boils down to solving the zeros of the associated characteristic polynomial (**art.** 138). In addition, we know (**art.** 1), due to symmetry of A, that all zeros are real, a fact that considerably simplifies matters as shown in Chapter 9. For, nearly all of the polynomials with real coefficients possess complex zeros, and only a very small subset has zeros that are all real. This suggests that there must be something special about these eigenvalues and characteristic polynomials of A. There is one most fascinating class of polynomials with real coefficients whose zeros are all real: orthogonal polynomials, which are studied in Chapter 10. In some particular cases, there is, indeed, a relation between the spectrum (eigenvalues) of the graph and the zeros of orthogonal polynomials.

Much of the research in the spectral analysis of graphs is devoted to understand

[2] Communicated to me by Dajie Liu.

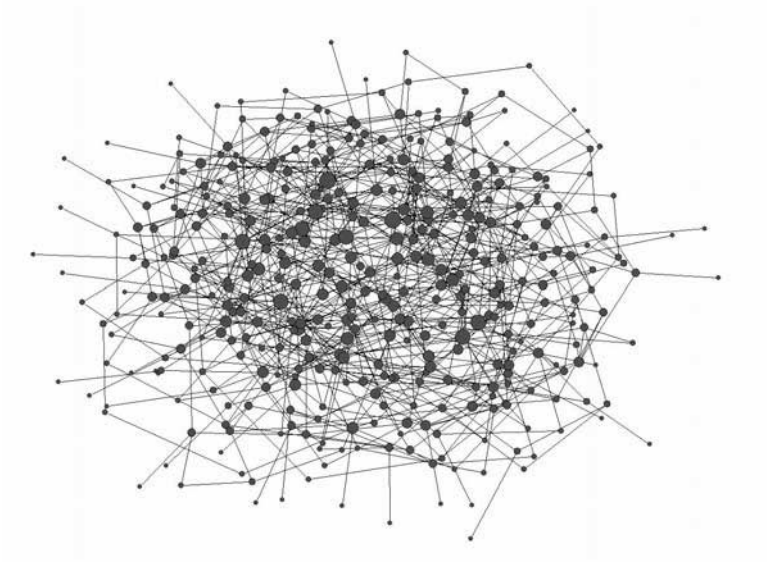

Fig. 1.1. A realization of an Erdős-Rényi random graph $G_p(N)$ with $N = 400$ nodes, $L = 793$ links and average degree $\frac{2L}{N}$ of about 4. The link density $p \simeq 10^{-2}$ equals the probability to have a link between two arbitrary chosen nodes in $G_p(N)$. The size of a node is drawn proportional to its degree.

properties of the graph by inspecting the spectra of mainly two matrices, the adjacency matrix A and the Laplacian Q, defined in **art.** 2. For example, how does the spectrum show that a graph is connected? What is the physical meaning of the largest and smallest eigenvalue, how large or small can they be? How are eigenvalues changing when nodes and/or links are added to the graph? Deeper questions are, "Is Λ alone, without X in (1.2), sufficient to characterize a graph?", "How are the spacings, the differences between consecutive eigenvalues, distributed and what do spacings physically mean?", or, extremal problems as "What is the class of graphs on N nodes and L links that achieves the largest second smallest eigenvalue of the Laplacian?", and so on.

1.2 Outline of the book

Chapter 2 introduces some definitions and concepts of algebraic graph theory, which are needed in Part I. We embark on the subject in Chapter 3 that focuses on the eigenvalues of the adjacency matrix A. In Chapter 4, we continue with the investigation of the spectrum of the Laplacian Q. As argued by Mohar, the theory of the Laplacian spectrum is richer and contains more beautiful achievements than that of the adjacency matrix. In Chapter 5, we compute the entire adjacency spectrum and sometimes also the Laplacian spectrum of special types of classes containing at least one variable parameter such as the number of nodes N or/and

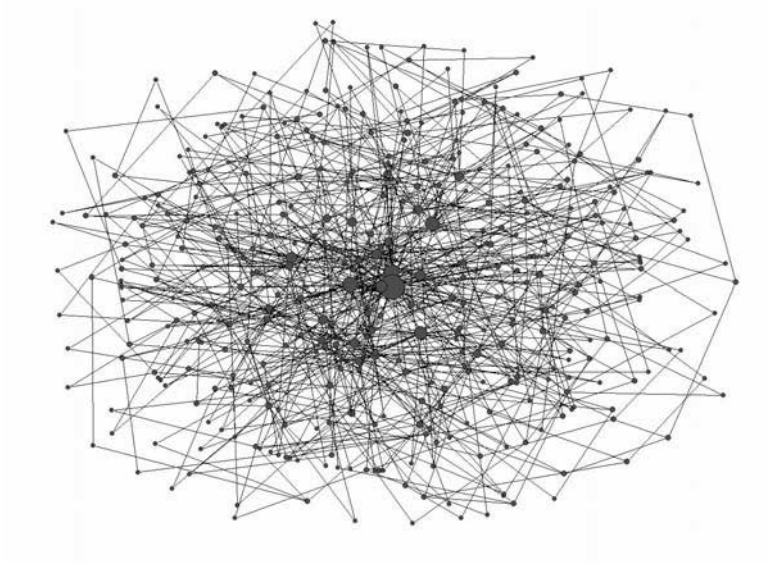

Fig. 1.2. An instance of a Barabási-Albert graph with $N = 400$ nodes and $L = 780$ links, which is about the same as in Fig. 1.1. The size of a node is drawn proportional to its degree.

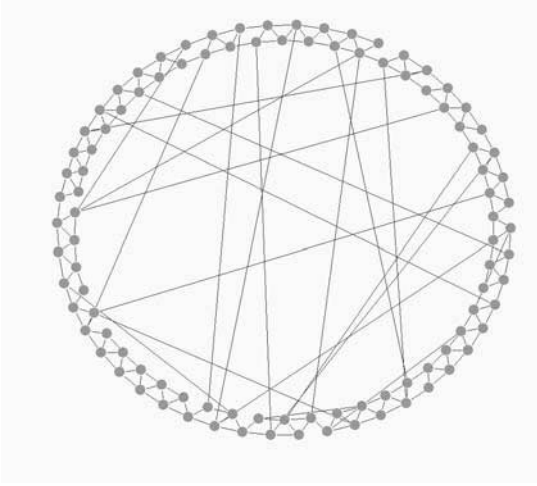

Fig. 1.3. The Watts-Strogatz small world graph on $N = 100$ nodes and with nodal degree $D = 4$ (or $k = 2$ as explained in Section 5.2) and rewiring probability $p_r = \frac{1}{100}$.

the number links L. This chapter thus illustrates the theory of Chapter 3 and Chapter 4 by useful examples. In fact, the book originated from Chapter 5 and it was a goal to collect all spectra of graphs (with at least one parameter that can be varied). The underlying thought was to explain the spectrum of a complex network

by features appearing in "known spectra". Chapter 6 complements Chapter 5 asymptotically when graphs grow large, $N \to \infty$. For large graphs, the density or distribution of the eigenvalues (as nearly continuous variables) is more appealing and informative than the long list of eigenvalues. Apart from the three marvelous scaling laws by Wigner, Marčenko-Pastur and McKay, we did not find many explicit results on densities of eigenvalues of graphs. Finally, Chapter 7, the last chapter of Part I, applies the spectral knowledge of the previous chapters to gain physical insight into the nature of complex networks.

As mentioned in the Preface, the results derived in Part I have been built on the general theory of linear algebra and of polynomials with real coefficients summarized in Part II.

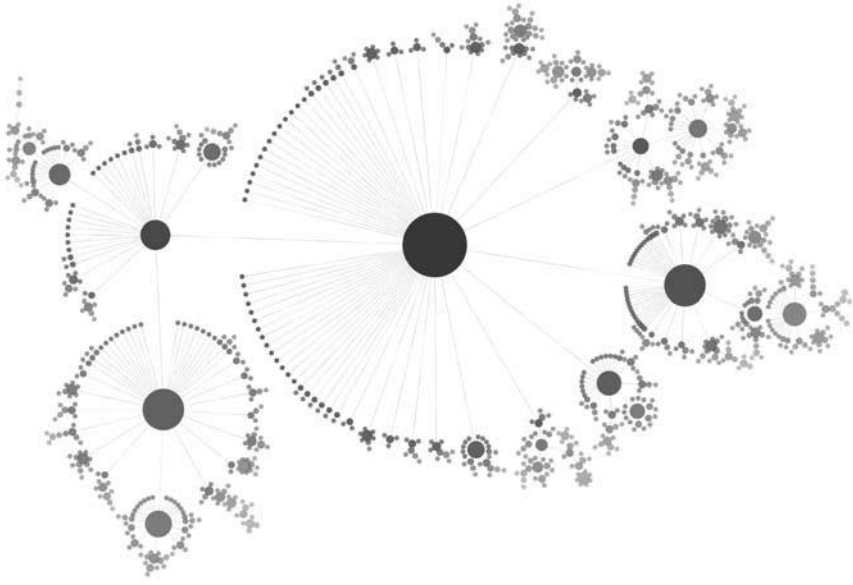

Fig. 1.4. A Barabási "fractal-like" tree with $N = 1000$ nodes, grown by adding at each step one new node to nodes already in the tree and proportional to their degree.

1.3 Classes of graphs

The main classes of graphs in the study of complex networks are: the class of Erdős-Rényi random graphs (Fig. 1.1), whose fascinating properties are derived in Bollobas (2001); the class of Watts-Strogatz small-world graphs (Fig. 1.3) first explored in Watts (1999); the class of Barabási-Albert power law graphs (Fig. 1.2 and Fig. 1.4) introduced by Barabási and Albert (1999); and the regular hyper-lattices in several dimensions.

The Erdős-Rényi random graph is the simplest random model for a network. Its

analytic tractability in a wide range of graph problems has resulted in the richest and most beautiful theory among classes of graphs. In many cases, the Erdős-Rényi random graph serves as a basic model that provides a fast benchmark for first order estimates and behaviors in real networks. Usually, if a graph problem cannot be solved analytically for the Erdős-Rényi random graph or for hyper-lattices, few hope exists that other classes of (random) graphs may have a solution. However, in particular the degree distribution of complex networks does not match well with the binomial degree distribution of Erdős-Rényi random graphs (drawn in Fig. 1.5) and this observation has spurred the search for "more realistic models".

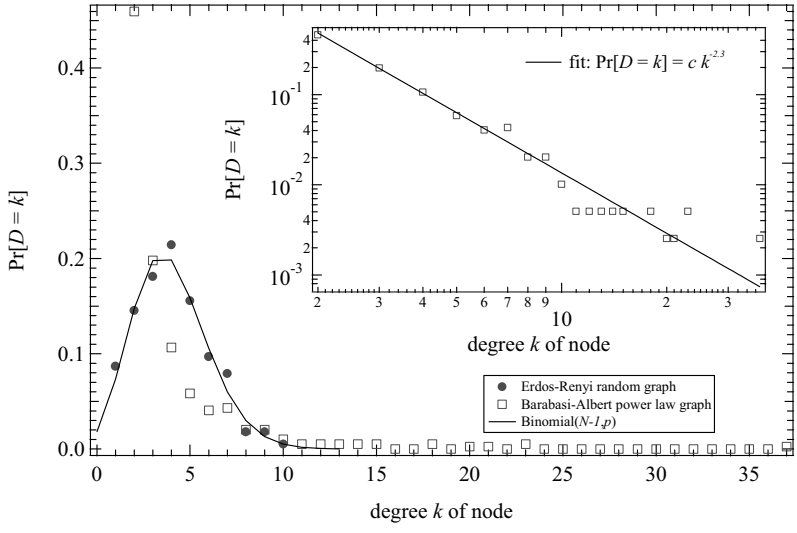

Fig. 1.5. The probability density function (pdf) of the nodal degree in the Erdős-Rényi random graph shown in Fig. 1.1 and in the Barabási-Albert power law graph in Fig. 1.2.

The Watts-Strogatz small-world graphs (after random rewiring of links) possesses a relatively high clustering and short hopcount. The probability p_r that a link is rewired seems to be a powerful tool in Watts-Strogatz small-world graphs to balance between "long hopcounts" (p_r is small) and "small-worlds" ($p_r \to 1$).

The most distinguishing property of the Barabási-Albert power law graphs is the power law degree distribution, $\Pr[D = k] \approx ck^{-\tau}$ with power index $\tau \approx 3$ for large N where c is a normalization constant, which is observed as a major characteristic in many real-world complex networks. Fig. 1.5 compares the degree distribution of the Erdős-Rényi random graph shown in Fig. 1.1 and of the Barabási-Albert power law graph in Fig. 1.2, both with the same number of nodes ($N = 400$) and almost the same average degree ($E[D] = 4$). The insert illustrates the characteristic power law of the Barabási-Albert graph, recognized by a straight line in a log-log plot. Most nodes in the Barabási-Albert power law graph have small degree, while a few nodes have degree larger than 10 (which is the maximum degree in the

Erdős-Rényi random graph with same number of nodes and links), and even one node has 36 neighbors. A power law graph is often called a "scale-free graph", meaning that there is no typical scale for the degree. Thus, the standard deviation $\sigma_D = \sqrt{\mathrm{Var}\,[D]}$ is usually larger than the average $E\,[D]$, such that the latter is not a good estimate for the random variable D of the degree, in contrast to Gaussian or binomial distributions, where the bell-shape is centered around the mean with, usually, small variance. Physically, power law behavior can be explained by the notion of long-range dependence, heavy correlations over large spacial or temporal intervals, and of self-similarity. A property is self-similar if on various scales (in time or space) or aggregation levels (e.g., hierarchical structuring of nodes in a network) about the same behavior is observed. The result is that a local property is magnified or scaled-up towards a global extent. Mathematically, $\Pr\,[D = \alpha k] \approx c\alpha^{-\tau}k^{-\tau}$, from which $\Pr\left[\alpha^{-1}D = k\right] = \alpha^{-\tau}\Pr\,[D = k]$; scaling the property (here, the degree D) by a factor α^{-1} leads to precisely the same distribution, apart from a proportionality constant $\alpha^{-\tau}$. Thus, on different scales, the behavior "looks" similar.

There is also a large number of more dedicated classes, such as Ramanujan graphs and the Kautz graphs, shown in Fig. 1.6, that possess interesting extremal properties. We will not further elaborate on the different properties of these classes;

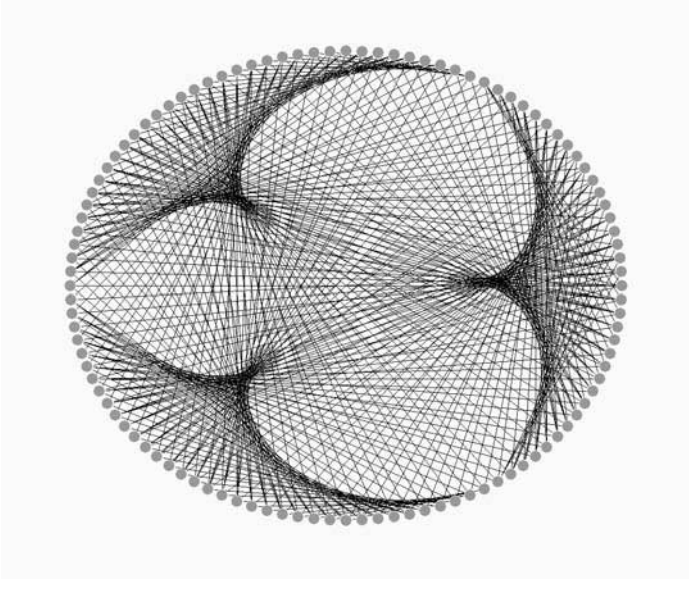

Fig. 1.6. The Kautz graph of degree $d = 3$ and of dimension $n = 3$ has $(d+1)\,d^n$ nodes and $(d+1)\,d^{n+1}$ links. The Kautz graph has the smallest diameter of any possible directed graph with N nodes and degree d.

we have merely included some of them here to illustrate that complex networks are

studied by comparing observed characteristics to those of "classes of graphs with known properties".

1.4 Outlook

I believe that we still do not understand "networks" sufficiently. For example, if the data (e.g., the adjacency matrix) of a large graph is given, and you are not allowed to visualize the network, it seems quite complex to tell, by computing graph metrics only, what the properties of the network are. You may list a large number of topological metrics such as hopcount, eccentricity, diameter, girth, expansion, betweenness, distortion, degree, assortativity, coreness, clique number, clustering coefficient, vertex and edge connectivity and others. We as humans see a pile of numbers, but often miss the overall picture and understanding.

I believe that the spectrum, that is for a sufficiently large graph a unique fingerprint as conjectured in van Dam and Haemers (2003), may reveal much more. First, graph or topology metrics are generally correlated and dependent. In contrast, eigenvalues weigh the importance of eigenvectors, that are all orthogonal, which makes the spectrum a more desirable device. Second, the belief in the spectrum stems from earlier research in condensed matter (Borghs *et al.*, 1989), where we have deduced from the photoluminescence spectra, quite useful and precise information about the structural properties of doped GaAs substrates. By inspecting long and carefully the differences in peaks and valleys, in gaps and in the broadness of the distribution of eigenvalues, that physically represented energy levels in the solid described by Schrödinger's equation in Section 1.1, insight gradually arose. A similar track may be followed to understand real, complex networks, because at the time of writing, "reading and understanding" the spectrum of a graph seems beyond our ability. We hope that the mathematical properties of spectra, presented here, may help in achieving this goal.