Graph Spectra
for Complex Networks

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GRAPH SPECTRA FOR COMPLEX NETWORKS

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to Saskia

who tolerated with love
that science is a passionate
and most demanding mistress

Contents

Preface

During the first years of the third millennium, considerable interest arose in com plex networks such as the Internet, the world wide web, biological networks, utility infrastructures (for transport of energy, waste, water, trains, cars and aircrafts), social networks, human brain networks, and so on. It was realized that complex networks are omnipresent and of crucial importance to humanity, whose still aug menting living standards increasingly depend on complex networks. Around the beginning of the new era, general laws such as "preferential attachment" and the "power law of the degree" were observed in many, totally different complex net works. This fascinating coincidence gave birth to an area of new research that is still continuing today. But, as is often the case in science, deeper investigations lead to more questions and to the conclusion that so little is understood of (large) networks. For example, the rather simple but highly relevant question "What is a robust network?" seems beyond the realm of present understanding. The most natural way to embark on solving the question consists of proposing a set of metrics that tend to specify and quantify "robustness". Soon one discovers that there is no universal set of metrics, and that the metrics of any set are dependent on each other and on the structure of the network.

Any complex network can be represented by a graph. Any graph can be repre sented by an adjacency matrix, from which other matrices such as the Laplacian are derived. These graph related matrices are defined in Chapter 2. One of the most beautiful aspects of linear algebra is the notion that, to each matrix, a set of eigenvalues with corresponding eigenvectors can be associated. The physical mean ing of an "eigen" system is best understood by regarding the matrix as a geometric transformation of "points" in a space. Those "points" define a vector: a line seg ment from an origin that ends in the particular point and that is directed from origin to end. The transformation (rotation, translation, scaling) of the vector is again a vector in the same space, but generally different from the original vector. The vector that after the transformation turns out to be proportional with itself is called an eigenvector and the proportionality strength or the scaling factor is the eigenvalue. The Dutch and German adjective "eigen" means something that is in herent to itself, a characteristic or fundamental property. Thus, knowing that each graph is represented by a matrix, it is natural to investigate the "eigensystem", the set of all eigenvalues with corresponding eigenvectors because the "eigensystem" characterizes the graph. Stronger even, since both the adjacency and Laplacian matrix are symmetric, there is a one to one correspondence between the matrix and the "eigensystem", established in **art.** 151.

In a broader context, transformations have proved very fruitful in science. The

most prominent is undoubtedly the Fourier (or Laplace) transform. Many branches
of science ranging from mathematics, physics and engineering abound with exam
ples that show the power and beauty of the Fourier transform. The general principle
of such transforms is that one may study the problem in either of two domains:
in the original one and in the domain after transformation, and that there exists
a one to one correspondence between both domains. For example, a signal is a
continuous function of time that may represent a message or some information pro
duced over time. Some properties of the signal are more appropriately studied in
the time domain, while others are in the transformed domain, the frequency do
main. This analogy motivates us to investigate some properties of a graph in the
topology domain, represented by a graph consisting of a set of nodes connected by
a set of links, while other properties may be more conveniently dealt with in the
spectral domain, specified by the set of eigenvalues and eigenvectors.

The duality between topology and spectral domain is, of course, not new and
has been studied in the field of mathematics called *algebraic graph theory*. Several
books on the topic, for example by Cvetković *et al.* (1995); Biggs (1996); Godsil
and Royle (2001) and recently by Cvetković *et al.* (2009), have already appeared.
Notwithstanding these books, the present one is different in a few aspects. First, I
have tried to build up the theory as a connected set of basic building blocks, called
articles, which are abbreviated by **art.** The presentation in article style was inspired
by great scholars in past, such as Gauss (1801) in his great treatise *Disquisitiones
Arithmeticae*, Titchmarsh (1964) in his *Theory of Functions*, and Hardy and Wright
(1968) in their splendid *Introduction to the Theory of Numbers*, and many others
that cannot be mentioned all. To some extent, it is a turning back to the past,
where books were written for peers, and without exercise sections, which currently
seem standard in almost all books. Thus, this book does not contain exercises.
Second, the book focuses on general theory that applies to all graphs, and much
less to particular graphs with special properties, of which the Petersen graph, shown
in Fig. 2.3, is perhaps the champion among all. In that aspect, the book does not
deal with a zoo of special graphs and their properties, but confines itself to a few
classes of graphs that depend at least on a single parameter, such as the number
of nodes, that can be varied. Complex networks all differ and vary in at least some
parameters. Less justifiable is the omission of multigraphs, directed graphs and
weighted graphs. Third, I have attempted to make the book as self contained as
possible and, as a peculiar consequence, the original appendices consumed about
half of the book! Thus, I decided to create two parts, the main part I on the
spectra, while part II overviews interesting results in linear algebra and the theory
of polynomials that are used in part I. Since each chapter in part II discusses a wide
area in mathematics, in fact, separate books on each topic are required. Hence, only
the basic theory is discussed, while advanced topics are not covered, because the
goal to include part II was to support part I. Beside being supportive, part II
contains interesting theory that opens possibilities to advance spectral results. For
example, Laguerre's beautiful Theorem 51 may once be applied to the characteristic

polynomials of a class of graphs with the same number of negative, positive and zero eigenvalues of the adjacency matrix.

A drawback is that the book does not contain a detailed list of references pointing to the original, first published papers: it was not my intention to survey the literature on the spectra of graphs, but rather to write a cohesive manuscript on results and on methodology. Sometimes, different methods or new proofs of a same result are presented. The monograph by Cvetković *et al.* (1995), complemented by Cvetković *et al.* (2009), still remains the invaluable source for references and tables of graph spectra.

The book is a temporal reflection of the current state of the art: during the process of writing, progress is being made. In particular, the many bounds that typify the field are continuously improved. The obvious expectation is that future progress will increasingly shape and fine tune the field into   hopefully   maturity. Hence, the book will surely need to be updated and all input is most welcome. Finally, I hope that the book may be of use to others and that it may stimulate and excite people to dive into the fascinating world of complex networks with the rigorous devices of algebraic graph theory offered here.

Ars mathematicae

October 2010 PIET VAN MIEGHEM

Acknowledgements

Symbols

Only when explicitly mentioned, will we deviate from the standard notation and symbols outlined here.

Random variables and matrices are written with capital letters, while complex, real, integer, etc., variables are in lower case. For example, X refers to a random variable, A to a matrix, whereas x is a real number and z is complex number. Usually, i, j, k, l, m, n are integers. Operations on random variables are denoted by [.], whereas (.) is used for real or complex variables. A set of elements is embraced by {.}.

Linear algebra

A $\qquad$ $n \times m$ matrix $\begin{bmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & & \\ a_{n1} & \cdots & a_{nm} \end{bmatrix}$

$\det A$ $\qquad$ determinant of a square matrix A; also denoted by $\begin{vmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \\ a_{n1} & \cdots & a_{nn} \end{vmatrix}$

$\text{trace}(A)$ $\quad = \sum_{j=1}^{n} a_{jj}$: sum of diagonal elements of A

$\text{diag}(a_k)$ $\quad = \text{diag}(a_1, a_2, \ldots, a_n)$: a diagonal matrix with diagonal elements listed, while all off diagonal elements are zero

A^T $\qquad$ transpose of a matrix, the rows of A are the columns of A^T

A^* $\qquad$ matrix in which each element is the complex conjugate of the corresponding element in A

A^H $\qquad = (A^*)^T$: Hermitian of matrix A

$c_A(x)$ $\qquad = \det(A - xI)$: characteristic polynomial of A

$\text{adj}A$ $\qquad = A^{-1} \det A$: adjugate of A

$Q(\lambda)$ $\qquad = \frac{c_A(\lambda)}{\lambda I - A}$: adjoint of A

e_j $\qquad$ basic vector, all components are zero, except for component j that is 1

δ_{kj} $\qquad$ Kronecker delta, $\delta_{kj} = 1$ if $k = j$, else $\delta_{kj} = 0$

Probability theory

$\Pr[X]$	probability of the event X
$E[X]$	$= \mu$: expectation of the random variable X
$\text{Var}[X]$	$= \sigma_X^2$: variance of the random variable X
$f_X(x)$	$= \frac{dF_X(x)}{dx}$: probability density function of X
$F_X(x)$	probability distribution function of X
$\varphi_X(z)$	probability generating function of X
	$\varphi_X(z) = E\left[z^X\right]$ when X is a discrete r.v.
	$\varphi_X(z) = E\left[e^{zX}\right]$ when X is a continuous r.v.
$\{X_k\}_{1\le k \le m}$	$= \{X_1, X_2, \ldots, X_m\}$
$X_{(k)}$	k th order statistics, k th smallest value in the set $\{X_k\}_{1\le k \le m}$
P	transition probability matrix (Markov process)
$1_{\{x\}}$	indicator function: $1_{\{x\}} = 1$ if the event or condition $\{x\}$ is true, else $1_{\{x\}} = 0$. For example, $\delta_{kj} = 1_{\{k=j\}}$

Graph theory

$\mathcal{L}$	set of links in a graph
$\mathcal{N}$	set of nodes in a graph
L	$= |\mathcal{L}|$: number of links in a graph
N	$= |\mathcal{N}|$: number of nodes in a graph
K_N	the complete graph with N nodes
$K_{n,m}$	the complete bi partite graph with $N = n + m$
d_j	degree of node j
$d_{(j)}$	the j th largest degree of node in a graph
$d_{\max}$	maximum degree in the graph
$d_{\min}$	minimum degree in the graph
D	degree in a graph (random variable)
$\kappa_{\mathcal{N}}(G)$	vertex (node) connectivity of graph G
$\kappa_{\mathcal{L}}(G)$	edge (link) connectivity of graph G
H	hopcount in a graph (random variable)
A	adjacency matrix of graph G
B	incidence matrix of graph G
Q	$= BB^T$ Laplacian matrix of graph G
J	all one matrix
u	all one vector
$\blacktriangle_G$	the number of triangles in G
Δ	$= \text{diag}(d_1, d_2, \ldots, d_N)$: diagonal matrix of the nodal degrees
$\{\lambda_k\}_{1\le k \le N}$	set of eigenvalues of A ordered as $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_N$
$\{\mu_k\}_{1\le k \le N}$	set of eigenvalues of Q ordered as $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_N$
N_k	total number of walks with length k
W_k	number of closed walks with length k

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

$$A = X\Lambda X^T \qquad (1.2)$$

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 na ture 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 eigen value 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 prop erty 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 differ ent "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. Al though 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

$$\lambda_k^2 (x_k)_j = \sum_{l_1=1}^{N} a_{jl_1} \sum_{l_2=1}^{N} a_{l_1 l_2} (x_k)_{l_2} = \sum_{l_2=1}^{N} \left(A^2\right)_{jl_2} (x_k)_{l_2}$$

$$= d_j (x_k)_j + \sum_{l_2 \text{ is a second hop neighbor of } j} (x_k)_{l_2}$$

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

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[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

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

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

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[2] Communicated to me by Dajie Liu.
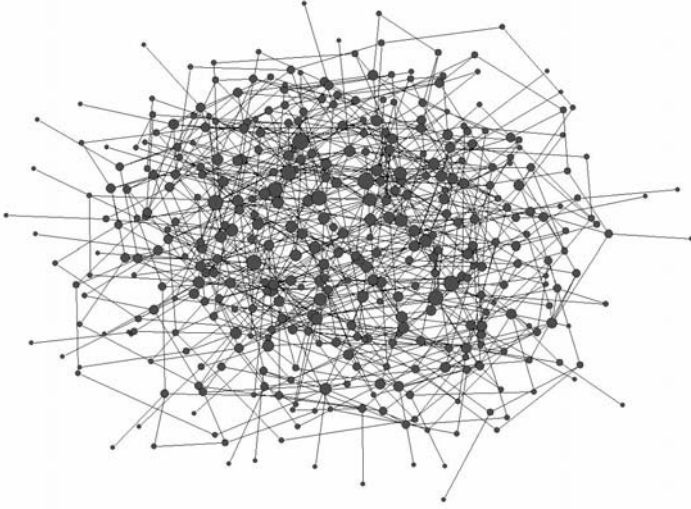
Fig. 1.1. A realization of an Erdős Rényi random graph $G_p(N)$ with $N = 400$ nodes, $L = 793$ links and average degree $\frac{2L}{N}$ of about 4. The link density $p \simeq 10^{-2}$ equals the probability to have a link between two arbitrary chosen nodes in $G_p(N)$. The size of a node is drawn proportional 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
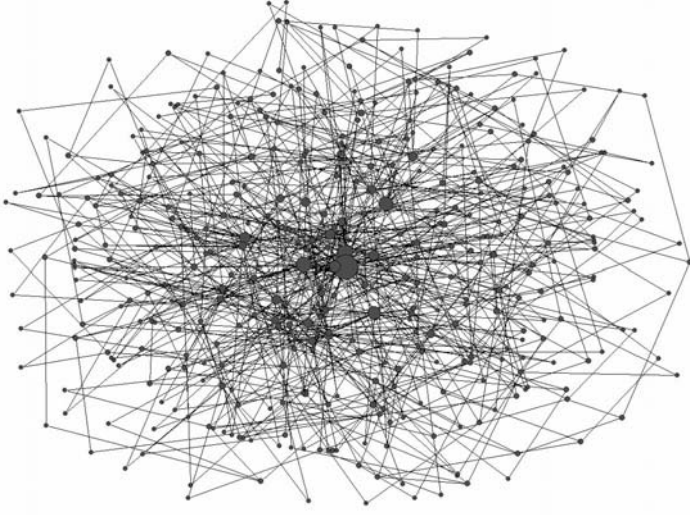
Fig. 1.2. An instance of a Barabási Albert graph with $N = 400$ nodes and $L = 780$ links, which is about the same as in Fig. 1.1. The size of a node is drawn proportional to its degree.
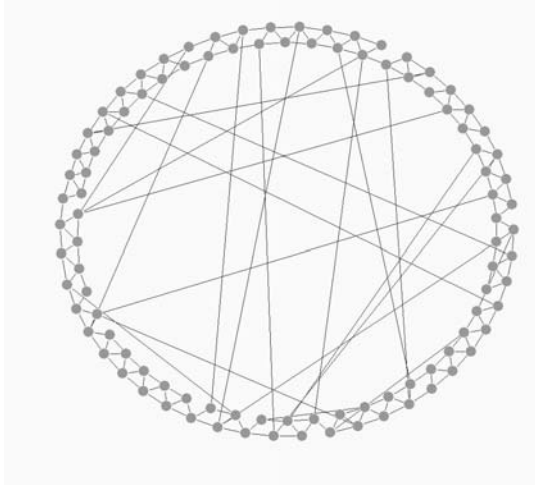
Fig. 1.3. The Watts Strogatz small world graph on $N = 100$ nodes and with nodal degree $D = 4$ (or $k = 2$ as explained in Section 5.2) and rewiring probability $p_r = \frac{1}{100}$.

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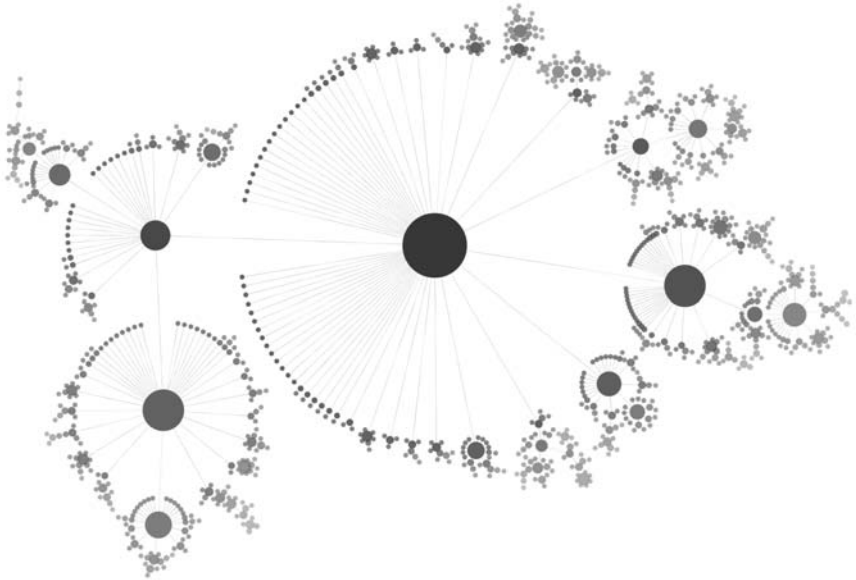
Fig. 1.4. A Barabási "fractal like" tree with $N = 1000$ nodes, grown by adding at each step one new node to nodes already in the tree and proportional to their degree.

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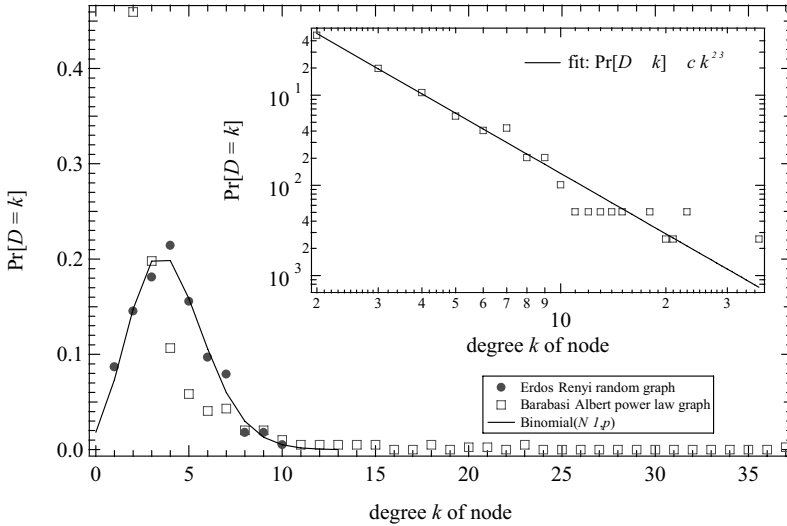
Fig. 1.5. The probability density function (pdf) of the nodal degree in the Erdős Rényi
random graph shown in Fig. 1.1 and in the Barabási Albert power law graph in Fig. 1.2.

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" ($p_r \rightarrow 1$).

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 $\Pr\,[\alpha^{-1} D = k] = \alpha^{-\tau} \Pr\,[D = k]$; 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;
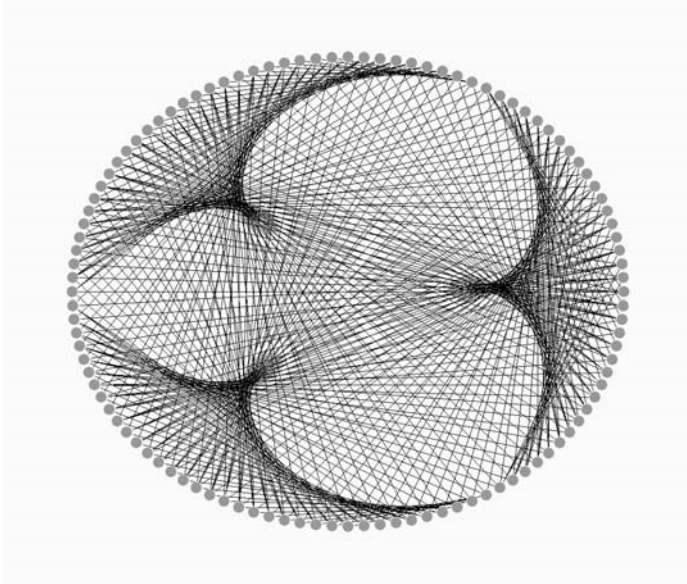
Fig. 1.6. The Kautz graph of degree $d = 3$ and of dimension $n = 3$ has $(d+1)\,d^n$ nodes and $(d+1)\,d^{n+1}$ links. The Kautz graph has the smallest diameter of any possible directed graph with N nodes and degree d.

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 fin gerprint as conjectured in van Dam and Haemers (2003), may reveal much more. First, graph or topology metrics are generally correlated and dependent. In con trast, eigenvalues weigh the importance of eigenvectors, that are all orthogonal, which makes the spectrum a more desirable device. Second, the belief in the spec trum stems from earlier research in condensed matter (Borghs *et al.*, 1989), where we have deduced from the photoluminescence spectra, quite useful and precise in formation 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.

Part I

Spectra of graphs

2

Algebraic graph theory

The elementary basics of the matrix theory for graphs $G(N, L)$ is outlined. The books by Cvetković *et al.* (1995) and Biggs (1996) are standard works on algebraic graph theory.

2.1 Graph related matrices

1. The *adjacency matrix* A of a graph G with N nodes is an $N \times N$ matrix with elements $a_{ij} = 1$ only if the pair of nodes (i, j) is connected by a link of G, otherwise $a_{ij} = 0$. If the graph is undirected, the existence of a link implies that $a_{ij} = a_{ji}$, the adjacency matrix $A = A^T$ is a real symmetric matrix. It is assumed further that the graph G does not contain self loops ($a_{ii} = 0$) nor multiple links between two nodes. The complement G^c of the graph G consists of the same set of nodes but with a link between (i, j) if there is *no* link (i, j) in G and vice versa. Thus, $(G^c)^c = G$ and the adjacency matrix A^c of the complement G^c is $A^c = J - I - A$ where J is the all one matrix ($(J)_{ij} = 1$). The links in a graph can be numbered
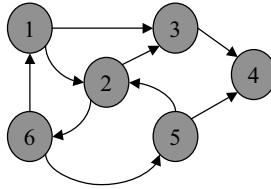
Fig. 2.1. A graph with $N = 6$ and $L = 9$. The links are lexicographically ordered, $e_1 = 1 \rightarrow 2, e_2 = 1 \rightarrow 3, e_3 = 1 \leftarrow 6$, etc.

in some way, for example, lexicographically as illustrated in Fig. 2.1. Information about the direction of the links is specified by the *incidence matrix* B, an $N \times L$ matrix with elements

$$b_{il} = \begin{cases} 1 & \text{if link } e_l = i \longrightarrow j \\ -1 & \text{if link } e_l = i \longleftarrow j \\ 0 & \text{otherwise} \end{cases}$$

Fig. 2.1 exemplifies the definition of A and B:

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

An important property of the incidence matrix B is that the sum of the columns equals zero,

$$u^T B = 0 \tag{2.1}$$

where $u = (1, 1, \ldots, 1)$ is the all one vector.

An undirected graph can be represented by an $N \times (2L)$ incidence matrix B, where each link (i, j) is counted twice, once for the direction $i \to j$ and once for the direction $j \to i$. In that case, the degree of each node is just doubled. Instead of using the incidence matrix, the unsigned incidence matrix R, defined in **art. 7**, can be more appropriate.

2. The relation between adjacency and incidence matrix is given by the *admittance* matrix or *Laplacian Q*,

$$Q = BB^T = \Delta - A$$

where $\Delta = \mathrm{diag}(d_1, d_2, \ldots, d_N)$ is the degree matrix. Indeed, if $i \neq j$ and noting that each column has precisely two non zero elements at a different row,

$$q_{ij} = \left(BB^T\right)_{ij} = \sum_{k=1}^{L} b_{ik} b_{jk} = \begin{cases} -1 & \text{if } (i, j) \text{ are linked} \\ 0 & \text{if } (i, j) \text{ are not linked} \end{cases}$$

If $i = j$, then $\sum_{k=1}^{L} b_{ik}^2 = d_i$, the number of links that have node i in common.

By the definition of A, the row sum i of A equals the degree d_i of node i,

$$d_i = \sum_{k=1}^{N} a_{ik} \tag{2.2}$$

Consequently, each row sum $\sum_{k=1}^{N} q_{ik} = 0$, which shows that Q is singular, implying that $\det Q = 0$.

Since $\sum_{i=1}^{N} \sum_{k=1}^{N} a_{ik} = 2L$, the basic law for the degree follows as

$$\sum_{i=1}^{N} d_i = 2L \tag{2.3}$$

Probabilistically, when considering an arbitrary nodal degree D thus, D is viewed as a random variable of the degree in a graph with possible realization or outcome equal to one of the values $d_1, d_2, \ldots, d_N$, the basic law for the degree equals

$$E[D] = \frac{2L}{N}$$

meaning that the average degree or expectation of D in any graph G is twice the ratio of the number L of links over the number N of nodes. Especially, in large real world networks, a probabilistic approach is adequate as illustrated in Section 7.

Let us define the degree vector $d = \begin{bmatrix} d_1 & d_2 & \cdots & d_N \end{bmatrix}^T$, then both (2.2) and (2.3) have a compact vector presentation as

$$Au = d \qquad (2.4)$$

and

$$u^T A u = d^T u = 2L \qquad (2.5)$$

3. Many other graph related matrices can be defined. We mention as an example the distance matrix H, where the element H_{ij} is equal to the shortest distance (in hops) between node i and node j and the modularity matrix M, defined in **art.** 104.

The matrix $P = \Delta^{-1}A$ is a stochastic matrix because all elements of P lie in the interval $[0, 1]$ and each row sum is 1.

Often weighted graphs are considered, defined by a non negative adjacency matrix W, where each element w_{ij} represents the weight of a link between node i and j and $w_{jj} = 0$ for all $1 \le j \le N$. A particular class of weighted graphs are undirected weighted graphs, where $W = W^T$. Similarly, the corresponding weighted Laplacian can be defined as $\tilde{Q} = \text{diag}\left(\sum_{j=1}^{N} w_{ij}\right) - W$, thus $\tilde{q}_{ij} = -w_{ij}$ if $i \ne j$, else, $\tilde{q}_{jj} = -\sum_{i=1;i\ne j}^{N} \tilde{q}_{ji}$.

2.1.1 The incidence matrix B

The $N \times L$ incidence matrix B transforms a $L \times 1$ vector y of the "link" space to a $N \times 1$ vector x of the "nodal" space by $x = By$. Physically, this transformation is best understood when y is a flow or current vector in a network. Then, the row $(By)_i = \sum_{k=1}^{L} B_{ik}y_k = x_i$ equals the sum of the in flows and out flows at node i. Left multiplying both sides of $x = By$ by u^T and using (2.1) yields $u^T x = 0$, which means that the net flow, influx plus outflow, in the network is zero. Thus, $By = x$ reflects a conservation law: the demand x_i offered at node i in the network is balanced by the sum of currents or flows at node i and the net demand or influx (outflow) to the network is zero.

4. *Rank of the incidence matrix B.*

Theorem 1 *If the network G is connected, then rank$(B) = N - 1$.*

Proof: The basic property (2.1) implies that rank$(B) \le N - 1$. Suppose that there exists a non zero vector $x \ne \alpha u$ for any real number α such that $x^T B = 0$. Under that assumption, the vector u and x are independent and the kernel (or zero space of B) consisting of all vectors v such that $v^T B = 0$ has at least rank 2,

and consequently $\text{rank}(B) \leq N - 2$. We will show that x is not independent, but proportional to u. Consider row j in B corresponding to the non zero component x_j. All non zero elements in the row vector $(B)_j$ are links incident to node j. Since each column of B only consists of two elements (with opposite signs), for each link l incident to node j, there is precisely one other row k in B with a non zero element in column l. In order for the linear relation $x^T B = 0$ to hold, we thus conclude that $x_j = x_k$, and this observation holds for all nodal indices j and k because G is connected. This implies that $x^T B = \alpha u^T B$, which shows that the rank of the incidence matrix cannot be lower than $N - 1$. □

An immediate consequence is that $\text{rank}(B) = N - k$ if the graph has k disjoint but connected components, because then (see also **art.** 80) there exists a relabeling of the nodes such that B can be partitioned as

$$
B = \begin{bmatrix}
B_1 & O & \cdots & O \\
O & B_2 & & \vdots \\
\vdots & & \ddots & \\
O & & \cdots & B_k
\end{bmatrix}
$$

5. *The cycle space and cut space of a graph G.* The cycle space of a graph G consists of all possible cycles in that graph. A cycle[1] of length k from node i back to node i is a succession of k undirected links of the form $(n_0 - n_1)(n_1 - n_2) \cdots (n_{k-1} - n_0)$, where $n_0 = i$. A cycle can have two cycle orientations. This means that the orientation of links in a cycle either coincides with the cycle orientation or that it is the reverse of the cycle orientation. For example, the cycle $(1 - 2)(2 - 6)(6 - 1)$ in Fig. 2.1 corresponds to the links (columns in B) $1, 3$ and 6 and all links are oriented in a same direction along the cycle. When adding columns $1, 3$ and 6, the sum is zero, which is equivalent to $By = 0$ with $y = (1, 0, 1, 0, 0, 1, 0, 0, 0)$. On the other hand, the cycle $(1 - 2)(2 - 3)(3 - 1)$ corresponds to the links $1, 2$ and 4, but not all links are oriented in the same direction such that $y = (1, -1, 0, 1, 0, 0, 0, 0, 0)$ has now negative sign components. In general, if $By = 0$, then the non zero components of the vector y are links of a cycle. Indeed, consider the j th row $(By)_j = x_j$. If node j is not incident with links of the cycle, then $x_j = 0$. If node j is incident with some links of the cycle, then it is incident with precisely two links, with opposite sign such that x_j is again zero.

Since the rank of B is $N - k$ (where k is the number of connected components), the rank of the kernel (or null space) of B is $L - N + k$. Hence, the dimension of the cycle space of a graph equals the rank of the kernel of B, which is $L - N + k$. The orthogonal complement of cycle space is called the cut space, with dimension $N - k$. Thus, the cut space is the space consisting of all vectors y for which $By = x \neq 0$. Since $u^T x = 0$, the non negative components of x are the nodes belonging to one

---

[1] **Art.** 17 defines a walk, from which it follows that a cycle is a closed walk, but a cycle is slightly more because the direction of a link $(n_k \quad n_{k+1})$ can be either $(n_k \to n_{k+1})$ or $(n_k \leftarrow n_{k+1})$.

partition and the negative components define the other partition. These two disjoint sets (or partitions) of nodes thus define a cut in the graph. For example in Fig. 2.1, $Bu = \begin{bmatrix} 1 & 0 & -1 & -2 & 1 & 1 \end{bmatrix}$ defines a cut that separates nodes 3 and 4 from the rest. Section 4.3 further investigates the partitioning of a graph.

6. *Spanning trees and the incidence matrix B.* Consider the incidence matrix B of a graph G and remove an arbitrary row in B, corresponding to a node n. Let M_n be one of the $\binom{L}{N-1}$ square $(N-1) \times (N-1)$ submatrices of B without row n and let G_n denote the subgraph of G on $N-1$ nodes formed by the links in the columns of M_n. Since there are $N-1$ columns in M_n, the subgraph G_n has precisely $N-1$ links, where some links may start or end at node n, outside the node set of G_n. We will now investigate $\det M_n$.

(a) Suppose first that there is no node with degree 1 in G, except possibly for n, in which case G_n is not a tree spanning $N-1$ nodes. Since the number of links is $L(G_n) = N - 1$, the basic law of the degree (2.3) shows that there must be a zero degree node in G_n. If the zero degree node is not n, then G_n has a zero row and $\det M_n = 0$. If n is the zero degree node, then each column of M_n contains a 1 and -1. Thus, each row sum of M_n is zero and $\det M_n = 0$.

(b) In the other case, G_n has a node i with degree 1. Then, the i th row in G_n only has one non zero element, either 1 or -1. After expanding $\det M_n$ by this i th row, we obtain a new $(N-2) \times (N-2)$ determinant $M_{n;i}$ corresponding to the graph $G_{n;i}$, formed by the links in the columns of $M_{n;i}$. For $\det M_{n;i}$, we can repeat the analysis: either $G_{n;i}$ is not a tree spanning the $N-2$ nodes of G except for n and i, in which case $\det M_{n;i} = 0$ or $\det M_{n;i} = \pm \det M_{n;i;k}$.

Iterating this process shows that the determinant of any square $(N-1) \times (N-1)$ submatrix of B is either 0, when the corresponding graph formed by the links, corresponding to the columns in B is not a spanning tree, or ± 1, when that corresponding graph is a spanning tree. Thus, we have shown:

Theorem 2 (Poincaré) *The determinant of any square submatrix of the incidence matrix B is either 0, 1, or -1.*

If the determinant of any square submatrix of a matrix is 0, 1, or -1, then that matrix is said to be *totally unimodular*.

2.1.2 The line graph

7. The line graph $l(G)$ of the graph $G(N, L)$ has as set of nodes the links of G and two nodes in $l(G)$ are adjacent if and only if they have, as links in G, exactly one node of G in common. The line graph $l(G)$ of G is sometimes called the "dual graph" or the "derived graph" of G. For example, the line graph of the star $K_{1,n}$ is the complete graph K_n and the line graph of the example graph in Fig. 2.1 is drawn in Fig. 2.2.
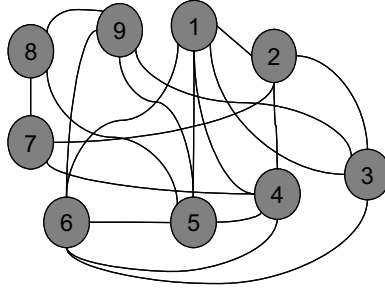
Fig. 2.2. The line graph of the graph drawn in Fig. 2.1.

We denote by R the absolute value of the incidence matrix B, i.e., $r_{ij} = |b_{ij}|$. In other words, $r_{ij} = 1$ if node i and link j are incident, otherwise $r_{ij} = 0$. Hence, the unsigned incidence matrix R ignores the direction of links in the graph, in contrast to the incidence matrix B. Analogous the definition of the Laplacian in **art. 2**, we may verify that the $N \times N$ adjacency matrix A of the graph G is written in terms of the unsigned $N \times L$ node link incidence matrix R as

$$A = RR^T - \Delta \tag{2.6}$$

The $L \times L$ adjacency matrix of the line graph $l(G)$ is similarly written in terms of R as

$$A_{l(G)} = R^T R - 2I \tag{2.7}$$

We remark that $B^T B$ is generally a $(-1, 0, 1)$ matrix, and that taking the absolute value of its entries equals $R^T R$, whereas the Laplacian matrix $Q = 2\Delta - RR^T = BB^T$.

In a graph G, where multiple links with the same direction between two nodes are excluded, we consider

$$\left(B^T B\right)_{ij} = \sum_{n=1}^{N} b_{ni} b_{nj} = \begin{cases} 1 & \text{if both link } i \text{ and } j \text{ either start or end in node } n \\ -1 & \text{if either link } i \text{ or } j \text{ starts or ends in node } n \\ -2 & \text{if link } i \text{ and } j \text{ have two nodes in common} \end{cases}$$

The latter case, where $\left(B^T B\right)_{ij} = -2$, occurs for a bidirectional link between two nodes. When the links at each node of the graph G either all start or all end, we observe that $\left(B^T B\right)_{ij} = 1$ for all links i and j and, in that case, there holds that $B^T B = R^T R$. An interesting example of such a graph is the general bipartite graph, studied in Section 5.8, where the direction of the links is the same for each node in the set $\mathcal{M}$ to each node in the other set $\mathcal{N}$.

8. *Basic properties of the line graph.* The number of nodes in the line graph $l(G)$ equals L, the number of links in G. The number of links in the line graph $l(G)$ is computed from the basic law of the degree (2.5) and (2.7) with u the $L \times 1$ all one

vector as

$$L_{l(G)} = \frac{1}{2}u^T A_{l(G)} u = \frac{1}{2}u^T R^T R u - u^T u$$
$$= \frac{1}{2}\|Ru\|_2^2 - L$$

It follows from the definition of the unsigned incidence matrix R that $u_{1\times N}^T R = 2u_{L\times 1}^T$, which is the companion of (2.1), and that $Ru = d$, because the row sum of $\sum_{l=1}^{L} R_{il} = d_i$, the number of links in G incident to node i. Hence, we find that the number of links in the line graph $l(G)$ equals

$$L_{l(G)} = \frac{1}{2}d^T d - L = \frac{1}{2}\sum_{i=1}^{N} d_i^2 - L \tag{2.8}$$

Alternatively, each node i in G with degree d_i generates in the line graph $l(G)$ precisely d_i nodes that are all connected to each other (as in a clique), corresponding to $\binom{d_i}{2}$ links. The number of links in $l(G)$ is thus also $L_{l(G)} = \sum_{i=1}^{N} \binom{d_i}{2}$. **Art. 2** indicates that the average degree of a node in the line graph $l(G)$ is

$$E\left[D_{l(G)}\right] = \frac{2L_{l(G)}}{N_{l(G)}} = \frac{1}{L}\sum_{i=1}^{N} d_i^2 - 2$$

The degree vector of the line graph $l(G)$ follows from (2.4) as

$$d_{l(G)} = A_{l(G)} u_{L\times 1} = R^T R u - 2u$$
$$= R^T d - 2u$$

Since in each column of R (as in the incidence matrix B), there are only two non zero elements, the vector element $\left(R^T d\right)_l = d_{l+} + d_{l-}$, where l_+ denotes the node at the start and l_- the node at the end of the link l. Hence, the maximum (and similarly minimum) degree of the line graph $l(G)$ equals

$$\max d_{l(G)} = \max_{1\leq l\leq L} (d_{l+} + d_{l-} - 2) \leq d_{(1)} + d_{(2)} - 2$$

where $d_{(k)}$ denotes the k th largest degree in G.

When G is connected, then also $l(G)$ is connected as follows from the construction[2] (or definition) of the line graph $l(G)$.

Given a line graph $l(G)$, it is possible to reconstruct the original graph G. The reconstruction or the inverse $G = l^{-1}(l(G))$ is not so easy. Each link l in G connects two nodes i and j and is transformed in the line graph $l(G)$ to a node l that bridges two cliques K_{d_i} and K_{d_j}. If a line graph $l(G)$ can be partitioned into cliques, then the number of those cliques equals the number N of nodes in G and each node l in $l(G)$ that bridges two cliques i and j, corresponds to a link l in G between two nodes i and j. Apart from $G = K_3$, the reconstruction or inverse line graph $l^{-1}(G)$

---

[2] In a connected graph G, each node is reachable from any other node via a path (a sequence of adjacent links, **art. 17**). Similarly, in the dual setting corresponding to the line graph, each link in G is reachable from any other link via a path (a sequence of adjacent nodes or neighbors).

is unique. Algorithms to compute the original graph G from the line graph $l(G)$ are presented by Lehot (1974) and Roussopoulos (1973).

9. Since $R^T R$ is a Gram matrix (**art.** 175), all eigenvalues of $R^T R$ are non negative. Hence, it follows from (2.7) that the eigenvalues of the adjacency matrix of the line graph $l(G)$ are not smaller than -2.

   The adjacency spectra of the line graph $l(G)$ and of G are related by Lemma 10 since

$$\det\left(\left(R^T R\right)_{L \times L} - \lambda I\right) = \lambda^{L-N} \det\left(\left(R R^T\right)_{N \times N} - \lambda I\right)$$

Using the definitions (2.7) and (2.6) in **art.** 7 yields

$$\det\left(A_{l(G)} - (\lambda - 2) I\right) = \lambda^{L-N} \det\left(\Delta + A - \lambda I\right)$$

or

$$\det\left(A_{l(G)} - \lambda I\right) = (\lambda + 2)^{L-N} \det\left(\Delta + A - (\lambda + 2) I\right) \tag{2.9}$$

The eigenvalues of the adjacency matrix of the line graph $l(G)$ are those of the unsigned Laplacian $\Delta + A$ shifted over -2 and an eigenvalue at -2 with multiplicity $L - N$.

   If $B^T B = R^T R$, then we have by Lemma 10 that

$$\det\left(\left(B^T B\right)_{L \times L} - \lambda I\right) = \lambda^{L-N} \det\left(\left(B B^T\right)_{N \times N} - \lambda I\right)$$

from which

$$\det\left(Q - \lambda I\right) = \lambda^{N-L} \det\left(A_{l(G)} - (\lambda - 2) I\right)$$

or

$$\det\left(A_{l(G)} - \lambda I\right) = (\lambda + 2)^{L-N} \det\left(Q - (\lambda + 2) I\right) \tag{2.10}$$

In graphs G, where $B^T B = R^T R$, the eigenvalues of the adjacency matrix of the line graph $l(G)$ are those of the Laplacian $Q = \Delta - A$ shifted over -2 and an eigenvalue at -2 with multiplicity $L - N$.

   The restriction, that all eigenvalues of an adjacency matrix are not less than -2, is not sufficient to characterize line graphs (Biggs, 1996, p. 18). The state of the art knowledge about line graphs is reviewed by Cvetković *et al.* (2004), who treat the characterization of line graphs in detail. A graph is a line graph if it satisfies certain conditions. Referring for proofs to Cvetković *et al.* (1995, 2004), we mention here only:

Theorem 3 (Krausz) *A graph is a line graph if and only if its set of links can be partitioned into "non trivial" cliques such that (i) two cliques have at most one node in common and (ii) each node belongs to at most two cliques.*

Theorem 4 (Van Rooij and Wilf) *A graph is a line graph if and only if (i) it does not contain the star $K_{1,3}$ as an induced subgraph and (ii) the remaining (or*

opposite) nodes in any two triangles with a common link must be adjacent and each of such triangles must be connected to at least one other node in the graph by an odd number of links.

2.1.3 The quotient graph

10. *Permutation matrix P.* Consider the set $\mathcal{N} = \{n_1, n_2, \ldots, n_N\}$ of nodes of G, where n_j is the label of node j. The most straightforward way is the labeling $n_j = j$. Suppose that the nodes in G are relabeled. This means that there is a permutation, often denoted by π, that rearranges the node identifiers n_j as $n_i = \pi(n_j)$. The corresponding permutation matrix P has element $p_{ij} = 1$ if $n_i = \pi(n_j)$, and $p_{ij} = 0$ otherwise.

For example, the set of nodes $\{1, 2, 3, 4\}$ is permuted to the set $\{2, 4, 1, 3\}$ by the permutation matrix

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

If the vector $v = (1, 2, 3, 4)$, then $Pv = w$, where the permuted vector $w = (2, 4, 1, 3)$. Next, $Pw = z = (4, 3, 2, 1)$, then $Pz = y = (3, 1, 4, 2)$, and $Py = v$. Thus, $P^4 v = v$. This observation holds in general, $P^N v = v$ for each $N \times N$ permutation matrix P: each node can be relabeled to one of the $\{n_1, n_2, \ldots, n_N\}$ possible labels and the permutation matrix maps each time a label $n_j \to \pi(n_j) = n_i$, where, generally, $n_i \neq n_j$, else certain elements are not permuted[3]. After N relabelings, we arrive again at the initial labeling. The definition (8.77) of the determinant shows that $\det P = \pm 1$, because in each row there is precisely one non zero element equal to 1.

Another example of a permutation matrix is the unit shift relabeling transformation in Section 5.2.1.

11. *A permutation matrix P is an orthogonal matrix.* Since a permutation matrix P relabels a vector v to a vector $w = Pv$, both vectors v and w contain the same components, but in a different order (provided $P \neq I$), such that their norms (**art.** 161) are equal, $\|v\| = \|w\|$. Using the Euclidean norm $\|x\|_2^2 = x^T x$, the equality $v^T v = w^T w$ implies that $P^T P = I$, such that P is an orthogonal matrix (**art.** 151).

12. If G_1 and G_2 are two directed graphs on the same set of nodes, then they are called *isomorphic* if and only if there is a permutation matrix P such that $P^T A_{G_1} P = A_{G_2}$. Since permutation matrices are orthogonal, $P^{-1} = P^T$, the spectra of G_1 and G_2 are identical (**art.** 151) : the spectrum is an invariant of the isomorphism class of a graph.

---

[3] The special permutation $P = I$ does not, in fact, relabel nodes.

13. *Automorphism.* We investigate the effect of a permutation π of the nodal set $\mathcal{N}$ of a graph on the structure of the adjacency matrix A. Suppose that $n_i = \pi(n_j)$ and $n_k = \pi(n_l)$, then we have with the definition of P in **art. 10**,

$$(PA)_{il} = \sum_{m=1}^{N} p_{im}a_{ml} = a_{jl}$$

$$(AP)_{il} = \sum_{m=1}^{N} a_{im}p_{ml} = a_{ik}$$

In order for A and P to commute, i.e., $PA = AP$, we observe that, between each node pair (n_j, n_l) and its permutation $(\pi(n_j), \pi(n_l))$ there must be a link such that $a_{jl} = 1 = a_{ik}$. An *automorphism* of a graph is a permutation π of the nodal set $\mathcal{N}$ such that (n_i, n_j) is a link of G if and only if $(\pi(n_i), \pi(n_j))$ is a link of G. Hence, if the permutation π is an automorphism, then A and P commute.

The consequences for the spectrum of the adjacency matrix A are interesting. Suppose that x is an eigenvector of A belonging to the eigenvalue λ, then

$$APx = PAx = P\lambda x = \lambda Px$$

which implies that Px is also an eigenvector of A belonging to eigenvalue λ. If x and Px are linearly independent, then λ cannot be a simple eigenvalue. Thus, an automorphism produces multiple eigenvectors belonging to a same eigenvalue.

14. *Partitions.* A generalization of a permutation is a partition that separates the nodal set $\mathcal{N}$ of a graph in disjoint, non empty subsets of $\mathcal{N}$, whose union is $\mathcal{N}$. The $k \in [1, N]$ disjoint, non empty subsets generated by a partition are sometimes called cells, and denoted by $\{C_1, C_2, \ldots, C_k\}$. If $k = N$, the partition reduces to a permutation. We also denote a partition by π.

Let $\{C_1, C_2, \ldots, C_k\}$ be a partition of the set $\mathcal{N} = \{1, 2, \ldots, N\}$ of nodes and let A be a symmetric matrix, that is partitioned as

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,k} \\ \vdots & & \vdots \\ A_{k,1} & \cdots & A_{k,k} \end{bmatrix}$$

where the block matrix $A_{i,j}$ is the submatrix of A formed by the rows in C_i and the columns in C_j. For example, the partition $C_1 = \{1, 3\}$, $C_2 = \{2, 4, 6\}$ and $C_3 = \{5\}$ of the nodes in Fig. 2.1 leads to the partitioned adjacency matrix

$$\pi A = \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} & \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \end{bmatrix} & \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} & [0] \end{bmatrix}$$

The characteristic matrix S of the partition, also called the community matrix S, is the $N \times k$ matrix whose columns are the vectors C_k labeled in accordance with $_\pi A$. Thus, in the example, the matrix S corresponding to the partition $C_1 = \{1, 3\}$, $C_2 = \{2, 4, 6\}$ and $C_3 = \{5\}$ is

$$S = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} u_2 & 0 & 0 \\ 0 & u_3 & 0 \\ 0 & 0 & u_1 \end{bmatrix}$$

where u_j is the all one vector of dimension j. Clearly, $S^T S = \text{diag}(2, 3, 1)$.

In general, $S^T S = \text{diag}(|C_1|, |C_2|, \ldots, |C_k|)$, where $|C_k|$ equals the number of elements in the set C_k. Each row of S only contains one non zero element, which follows from the definition of a partition: a node can only belong to one cell (or community) of the partition and the union of all cells is again the complete set $\mathcal{N}$ of nodes. Thus, the elements of the $N \times k$ community matrix S are

$$S_{ij} = \begin{cases} 1 & \text{if node } i \text{ belongs to the set (or community) } C_j \\ 0 & \text{otherwise} \end{cases}$$

and, the columns of S are orthogonal and $\text{trace}(S^T S) = N$.

15. *Quotient matrix.* The quotient matrix corresponding to the partition specified by $\{C_1, C_2, \ldots, C_k\}$ is defined as the $k \times k$ matrix

$$A^\pi = \left(S^T S\right)^{-1} S^T \left(_\pi A\right) S \tag{2.11}$$

where $\left(S^T S\right)^{-1} = \text{diag}\left(\frac{1}{|C_1|}, \frac{1}{|C_2|}, \ldots, \frac{1}{|C_k|}\right)$. The quotient matrix of the matrix A of the example in **art.** 14 is

$$A^\pi = \begin{bmatrix} 1 & 2 & 0 \\ \frac{4}{3} & \frac{2}{3} & 1 \\ 0 & 3 & 0 \end{bmatrix}$$

We can verify that $(A^\pi)_{ij}$ denotes the average row sum of the block matrix $(_\pi A)_{i,j}$. An example of the quotient matrix Q^π of a Laplacian Q is given in Section 5.11.

If the row sum of each block matrix $A_{i,j}$ is constant, then the partition π is called *equitable* (or regular). In that case, $A_{i,j} u = (_\pi A)_{i,j} u$ or $_\pi A S = S A^\pi$. Also, a partition π is equitable if, for any i and j, the number of neighbors that a node in C_i has in the cell C_j does not depend on the choice of a node in C_i. For example, consider a node v in the Petersen graph shown in Fig. 2.3 and construct the three cell partitions as $C_1 = \{v\}$, C_2 is the set of the neighbors of v and C_3 is the set of nodes two hops away from v.

The number of neighbors of v in C_2 is three and zero in C_3, while the number of
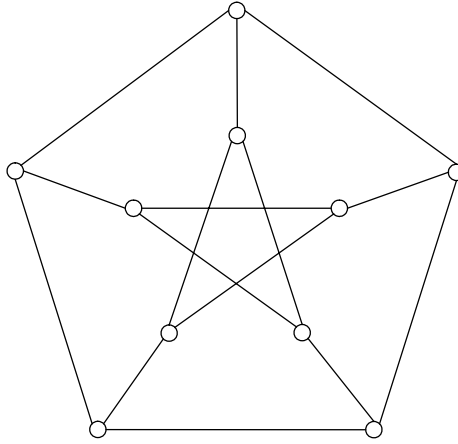
Fig. 2.3. The Petersen graph.

neighbors of a node in C_2 with C_3 is two such that

$$A^\pi = \begin{bmatrix} 0 & 3 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix}$$

A distance partition with respect to node v is the partition of $\mathcal{N}$ into the sets of nodes in G at distance r from a node v. A distance partition is, in general, not equitable.

If v is an eigenvector of A^π belonging to the eigenvalue λ, then Sv is an eigen vector of $_\pi A$ belonging to the same eigenvalue λ. Indeed, left multiplication of the eigenvalue equation $A^\pi v = \lambda v$ by S yields

$$\lambda Sv = SA^\pi v = (_\pi A) Sv$$

This property makes equitable partitions quite powerful.

For example, the adjacency matrix of the complete bipartite graph $K_{m,n}$ (see Section 5.7) has an equitable partition with $k = 2$. The corresponding quotient matrix is $A^\pi = \begin{bmatrix} 0 & m \\ n & 0 \end{bmatrix}$ whose eigenvalues are $\pm\sqrt{mn}$, which are the non zero eigenvalues of $K_{m,n}$. The quotient matrix of the complete multi partite graph is derived in Section 5.9.

The quotient graph of an equitable partition, denoted by G^π, is the directed graph with the cells of the partition π as its nodes and with $(A^\pi)_{ij}$ links going from cell/node C_i to node C_j. Thus, $(A^\pi)_{ij}$ equals the number of links that join a node in the cell C_i to the nodes in cell C_j. In general, the quotient graph contains multiple links and self loops. The subgraph induced by each cell in an equitable partition is necessarily a regular graph because each node in cell C_i has the same number of neighbors in cell C_j.

16. *Trees.* We consider an application of equitable partitions to trees. A tree T is *centrally symmetric* with center u if and only if there is an automorphism of T, which fixes u and which maps x to y, where x and y are any two nodes in T at the same distance from u.

Lemma 1 *A tree is centrally symmetric with respect to node u if and only if the distance partition is equitable.*

Proof: see Godsil (1993). □

Lemma 2 *Any tree with maximum degree $d_{\max}$ is a subgraph of a centrally sym metric tree $T_{d_{\max}}$ with property that all nodes of $T_{d_{\max}}$ have degree 1 or $d_{\max}$.*

Proof: see Godsil (1993). □

The tree $T_{d_{\max}}$ is completely determined once the radius, the distance from the center to an end node, is known. The quotient matrix A^π of the adjacency matrix of $T_{d_{\max}}$ corresponding to the distance partition is

$$
A^\pi = \begin{bmatrix}
0 & d_{\max} & 0 & \cdots & & 0 \\
1 & 0 & d_{\max}-1 & & & \\
 & & \ddots & & & \\
 & & 1 & 0 & d_{\max}-1 & \\
 & & & 1 & 0 &
\end{bmatrix}
$$

A similarity transform does not alter the eigenvalues (**art.** 142). If

$$
H = \operatorname{diag}\left(\left\{ \left(\sqrt{d_{\max}-1} \right)^i \ 1 \right\}_i \right)
$$

with the same dimensions as A^π, then $\widetilde{A^\pi} = H A^\pi H^{\ 1}$,

$$
\widetilde{A^\pi} = \begin{bmatrix}
0 & \frac{d_{\max}}{\sqrt{d_{\max}\ 1}} & 0 & \cdots & & 0 \\
\sqrt{d_{\max}-1} & 0 & \sqrt{d_{\max}-1} & & & \\
 & & \ddots & & & \\
 & & \sqrt{d_{\max}-1} & 0 & \sqrt{d_{\max}-1} & \\
 & & & \sqrt{d_{\max}-1} & 0 &
\end{bmatrix}
$$

These results are used in **art.** 63.

2.2 Walks and paths

17. A walk of length k from node i to node j is a succession of k arcs of the form $(n_0 \to n_1)(n_1 \to n_2)\cdots(n_{k\ 1} \to n_k)$ where $n_0 = i$ and $n_k = j$. A path is a walk in which all vertices are different, i.e., $n_l \neq n_m$ for all $0 \leq l \neq m \leq k$. A closed walk of length k, also called a cycle of length k, is a walk that starts in node i and returns, after k hops, to that same node i.

Lemma 3 *The number of walks of length k from node i to node j is equal to the element $\left(A^k\right)_{ij}$.*

Proof (by induction): For $k = 1$, the number of walks of length 1 between state i and j equals the number of direct links between i and j, which is by definition the element a_{ij} in the adjacency matrix A. Suppose the lemma holds for $k - 1$. A walk of length k consists of a walk of length $k - 1$ from i to some vertex r which is adjacent to j. By the induction hypothesis, the number of walks of length $k - 1$ from i to r is $\left(A^{k-1}\right)_{ir}$ and the number of walks with length 1 from r to j equals a_{rj}. The total number of walks from i to j with length k then equals $\sum_{r=1}^{N} \left(A^{k-1}\right)_{ir} a_{rj} = \left(A^k\right)_{ij}$ (by the rules of matrix multiplication). $\qquad\square$

Explicitly,

$$\left(A^k\right)_{ij} = \sum_{r_1=1}^{N} \sum_{r_2=1}^{N} \cdots \sum_{r_{k-1}=1}^{N} a_{ir_1} a_{r_1 r_2} \cdots a_{r_{k-2} r_{k-1}} a_{r_{k-1} j} \tag{2.12}$$

18. The number of paths with k hops between node i and node j is, for $k > 1$ and $N > 2$,

$$X_k(i, j; N) = \sum_{r_1 \neq \{i,j\}} \sum_{r_2 \neq \{i,r_1,j\}} \cdots \sum_{r_{k-1} \neq \{i,r_1,\ldots,r_{k-2},j\}} a_{ir_1} a_{r_1 r_2} \cdots a_{r_{k-1} j}$$

while the number of paths with $k = 1$ hop between the node pair (i, j) is

$$X_1(i, j; N) = a_{ij}$$

Symmetry of the adjacency matrix A implies that $X_k(i, j; N) = X_k(j, i; N)$. The definition of a path restricts the first index r_1 to $N - 2$ possible values, the second r_2 to $N - 3$, etc., such that the maximum number of k hop paths, which is attained in the complete graph K_N, where $a_{ij} = 1$ for each link (i, j), equals

$$\prod_{l=1}^{k-1} (N - 1 - l) = \frac{(N - 2)!}{(N - k - 1)!}$$

whereas the total possible number of walks follows from (2.12) as N^{k-1}.

The total number of paths M_N between two nodes in the complete graph is

$$M_N = \sum_{j=1}^{N-1} \frac{(N - 2)!}{(N - j - 1)!} = (N - 2)! \sum_{k=0}^{N-2} \frac{1}{k!}$$
$$= (N - 2)! e - R$$

where

$$R = (N-2)! \sum_{j=N_1}^{\infty} \frac{1}{j!} = \sum_{j=0}^{\infty} \frac{(N-2)!}{(N-1+j)!}$$

$$= \frac{1}{N-1} + \frac{1}{(N-1)N} + \frac{1}{(N-1)N(N+1)} + \cdots$$

$$< \sum_{j=1}^{\infty} \left(\frac{1}{N-1}\right)^j = \frac{1}{N-2}$$

implying that for $N \geq 3$, $R < 1$. But M_N is an integer. Hence, the total number of paths in K_N is exactly equal to

$$M_N = [e(N-2)!] \tag{2.13}$$

where $e = 2.718\,281...$ and $[x]$ denotes the largest integer smaller than or equal to x. Since any graph is a subgraph of the complete graph, the maximum total number of paths between two nodes in any graph is upper bounded by $[e(N-2)!]$.

19. *Diameter of a graph.* A graph G is connected if there exists a walk between each pair of nodes in G. Lemma 3 shows that connectivity is equivalent to the existence of some integer $k > 0$ for which $(A^k)_{ij} \neq 0$ for each nodal pair (i,j). The lowest integer k for which $(A^k)_{ij} \neq 0$ for each pair (i,j) of nodes is called the *diameter* of the graph G. The diameter thus equals the length of the longest shortest hop path in G.

20. *A shortest path.* To each link $e_l = i \to j \in \mathcal{L}$ from node $i \in \mathcal{N}$ to node $j \in \mathcal{N}$ in the network, we assign a link weight $w(e_l) = w_{ij}$, a non negative real number, which quantifies a property of that link such as the delay incurred or energy needed when traveling over that link, the distance, the capacity, monetary cost, etc. The set of all link weights is called the *link weight structure* of G. We consider only additive link weights such that the weight of a path P is $w(P) = \sum_{e_l \in P} w(e_l)$, i.e., $w(P)$ equals the sum of the weights of the constituent links of P. The shortest path $P_{A \to B}^*$ from A to B is the path with minimal weight, thus, $w(P_{A \to B}^*) \leq w(P_{A \to B})$ for all $P_{A \to B}$. If all link weights are equal to $w_{ij} = 1$, shortest paths are shortest hop paths and $w(P_{A \to B}^*)$ is also called the *distance* between nodes A and B.

There exist many routing algorithms to compute shortest paths in networks. The most important of these routing algorithms are explained, for example, in Van Mieghem (2006a) and Cormen *et al.* (1991).

3

Eigenvalues of the adjacency matrix

Only general results of the eigenvalue spectrum of a graph G are treated. For special types of graphs, there exists a wealth of additional, but specific properties of the eigenvalues.

3.1 General properties

21. Since A is a real symmetric matrix, **art.** 151 shows that A has N real eigenvalues, which we order as $\lambda_N \leq \lambda_{N-1} \leq \cdots \leq \lambda_1$. Apart from a similarity transform (**art.** 142), the set of eigenvalues with corresponding eigenvectors is unique. A similarity transform consists of a relabeling of the nodes in the graph that obviously does not alter the structure of the graph but merely expresses the eigenvectors in a different base.

The classical Perron Frobenius Theorem 38 in **art.** 168 for non negative square matrices states that λ_1 is a simple and non negative root of the characteristic polynomial in (8.3) possessing the only eigenvector of A with non negative components. The largest eigenvalue λ_1 is also called the *spectral radius* of the graph.

22. Since the characteristic polynomial $c_A(\lambda) = \det(A - \lambda I)$, defined in **art.** 138, has integer coefficients and $c_n = (-1)^N$, it follows from **art.** 197 that the only rational zeros of $c_A(\lambda)$, i.e., zeros belonging to $\mathbb{Q}$, are integers. This property also holds for the Laplacian matrix Q. For example, $\frac{3}{4}$ is never an eigenvalue of A nor Q.

23. Gerschgorin's Theorem 36 applied to the adjacency matrix states that any eigenvalue of A lies in the interval $[-d_{\max}, d_{\max}]$. Hence, $\lambda_1 \leq N - 1$ and this maximum is attained in the complete graph (see Section 5.1).

24. Theorem 63, with $m = 1$ and using (3.2), indicates that all the eigenvalues of A are contained in the interval $\left[-\sqrt{\frac{2(N-1)}{N}L}, \sqrt{\frac{2(N-1)}{N}L} \right]$.

25. Since $a_{ii} = 0$, we have that $\text{trace}(A) = 0$. From (8.7), the coefficient c_{N-1} of

the characteristic polynomial $c_A(\lambda)$ is

$$(-1)^{N-1} c_{N-1} = \sum_{k=1}^{N} \lambda_k = 0 \tag{3.1}$$

26. Applying the Newton identities (9.3) to the characteristic polynomial (8.3) and (8.5) of the adjacency matrix with $z_k = \lambda_k$, $a_k = (-1)^N c_k$ and $c_{N-1} = 0$ (from (3.1)) yields for the first few values,

$$c_{N-2} = -\frac{1}{2} \sum_{k=1}^{N} \lambda_k^2$$

$$c_{N-3} = -\frac{1}{3} \sum_{k=1}^{N} \lambda_k^3$$

$$c_{N-4} = \frac{1}{8} \left(\left(\sum_{k=1}^{N} \lambda_k^2 \right)^2 - 2 \sum_{k=1}^{N} \lambda_k^4 \right)$$

27. From (8.4), the coefficient of the characteristic polynomial $c_{N-2} = \sum_{\text{all}} M_2$. Each principal minor M_2 of the adjacency matrix A has a principal submatrix of the form $\begin{bmatrix} 0 & x \\ y & 0 \end{bmatrix}$ with $x, y \in [0, 1]$. A minor M_2 is non zero if and only if $x = y = 1$, in which case $M_2 = -1$. For each set of adjacent nodes, there exists a non zero minor, which implies that

$$c_{N-2} = -L$$

The Newton identities in **art.** 26 show that the number of links L equals

$$L = \frac{1}{2} \sum_{k=1}^{N} \lambda_k^2 \tag{3.2}$$

Since the mean $E[\lambda] = \frac{1}{N} \sum_{k=1}^{N} \lambda_k = 0$ (**art.** 25), the variance of the adjacency eigenvalues equals, invoking the basic law of the degree (2.3),

$$\text{Var}[\lambda] = \frac{1}{N} \sum_{k=1}^{N} \lambda_k^2 = \frac{2L}{N} = E[D]$$

Especially in order to understand the density function of the adjacency eigenvalues (for example, in Section 7), this stochastic interpretation is helpful.

28. Each principal submatrix $M_{3\times 3}$ of the adjacency matrix A is of the form

$$M_{3\times 3} = \begin{bmatrix} 0 & x & z \\ x & 0 & y \\ z & y & 0 \end{bmatrix}$$

and the corresponding minor $M_3 = \det M_{3\times 3} = 2xyz$ is only non zero for $x = y =$

$z = 1$. That form of $M_{3\times3}$ corresponds with a subgraph of three nodes that are fully connected. Hence, $c_{N\ 3} = -2\times$ the number of triangles $\blacktriangle_G$ in G. From **art. 26**, it follows that the number of triangles in G is

$$\blacktriangle_G = \frac{1}{6}\sum_{k=1}^{N}\lambda_k^3 \tag{3.3}$$

29. In general, from (8.4) and by identifying the structure of a minor M_k of A, any coefficient $c_{N\ k}$ can be expressed in terms of graph characteristics,

$$(-1)^N c_{N\ k} = \sum_{\mathcal{G}\in G_k}(-1)^{cycles(\mathcal{G})} \tag{3.4}$$

where G_k is the set of all subgraphs of G with exactly k nodes and $cycles\,(\mathcal{G})$ is the number of cycles in a subgraph $\mathcal{G} \in G_k$. The minor M_k is a determinant of the $M_{k\times k}$ submatrix of A and defined (see **art. 187**) as

$$M_k = \sum_{p}(-1)^{\sigma(p)}a_{1p_1}a_{2p_2}\cdots a_{kp_k}$$

where the sum is over all $k!$ permutations $p = (p_1, p_2, \ldots, p_k)$ of $(1, 2, \ldots, k)$ and $\sigma(p)$ is the parity of p, i.e., the number of interchanges of $(1, 2, \ldots, k)$ to obtain $(p_1, p_2, \ldots, p_k)$. Only if all the links $(1, p_1), (2, p_2), \ldots, (k, p_k)$ are contained in G, $a_{1p_1}a_{2p_2}\ldots a_{kp_k}$ is non zero. Since $a_{jj} = 0$, the sequence of contributing links $(1, p_1), (2, p_2), \ldots, (k, p_k)$ is a set of disjoint cycles such that each node in G_k belongs to exactly one of these cycles and $\sigma(p)$ depends on the number of those disjoint cycles. Now, M_k is constructed from a specific set $\mathcal{G} \in G_k$ of k out of N nodes and in total there are $\binom{N}{k}$ such sets in G_k. Combining all contributions leads to the expression (3.4).

Harary (1962) discusses the determinant $\det A$ of a directed graph, from which another expression than (3.4) for the coefficients c_k of the characteristic polynomial $c_A(\lambda)$ can be derived. An elementary subgraph of G on k nodes is a graph in which each component is either a link between two distinct nodes or a cycle. Here, a cycle is thus of at least length 3, possessing at least three nodes or links. Harary observes that, in the determinant of the adjacency matrix A (or in each of its minors) of a *directed* graph, each directed cycle of even (odd) length contributes negatively (positively) to $\det A$. Let e_c denote the number of even components in an elementary subgraph, i.e. containing an even number of nodes. Each cycle in an undirected graph corresponds to the two directions in its directed companion. Harary (1962) shows that the determinant of the adjacency matrix of an elementary subgraph $\mathcal{H}$ equals

$$\det A\,(\mathcal{H}) = (-1)^{e_c(\mathcal{H})}\, 2^{|c(\mathcal{H})|}\prod_{a_k\in e(\mathcal{H})}a_k^2\prod_{a_m\in c(\mathcal{H})}a_m$$

where $c\,(\mathcal{H})$ is the set of components that are cycles in $\mathcal{H}$ and $e\,(\mathcal{H})$ is the set of components that are simple links in $\mathcal{H}$. Finally, if H_k denotes the set of all

elementary subgraphs of G with k nodes, then the coefficient of the characteristic polynomial $c_A(\lambda)$ can be written as

$$(-1)^N c_{N\ k} = \sum_{\mathcal{H} \in H_k} (-1)^{e_c(\mathcal{H})} 2^{|c(\mathcal{H})|}$$

30. Since A is a symmetric 0 1 matrix, we observe that using (2.2),

$$\left(A^2\right)_{ii} = \sum_{k=1}^{N} a_{ik} a_{ki} = \sum_{k=1}^{N} a_{ik}^2 = \sum_{k=1}^{N} a_{ik} = d_i$$

Hence, with (3.2) and (8.7), the basic law for the degree (2.3) is expressed as

$$\text{trace}(A^2) = \sum_{k=1}^{N} \lambda_k^2 = \sum_{k=1}^{N} d_k = 2L \tag{3.5}$$

Furthermore,

$$\sum_{i=1}^{N} \sum_{j=1;j\neq i}^{N} \left(A^2\right)_{ij} = \sum_{i=1}^{N} \sum_{j=1;j\neq i}^{N} \sum_{k=1}^{N} a_{ik} a_{kj} = \sum_{k=1}^{N} \sum_{i=1}^{N} a_{ki} \sum_{j=1;j\neq i}^{N} a_{kj}$$

$$= \sum_{k=1}^{N} \sum_{i=1}^{N} a_{ki} (d_k - a_{ki}) = \sum_{k=1}^{N} \left(d_k \sum_{i=1}^{N} a_{ki} - \sum_{i=1}^{N} a_{ki} \right)$$

or

$$\sum_{i=1}^{N} \sum_{j=1;j\neq i}^{N} \left(A^2\right)_{ij} = \sum_{k=1}^{N} d_k (d_k - 1) \tag{3.6}$$

Lemma 3 states that $\sum_{i=1}^{N} \sum_{j=1;j\neq i}^{N} \left(A^2\right)_{ij}$ equals twice the total number of two hop walks with different source and destination nodes. In other words, the total number of connected triplets of nodes in G equals half (3.6). **Art.** 8 further shows that

$$\sum_{i=1}^{N} \sum_{j=1;j\neq i}^{N} \left(A^2\right)_{ij} = 2 \sum_{i=1}^{N} \binom{d_i}{2} = 2L_{l(G)}$$

which means that the number of links in the line graph $l(G)$ of the graph G equals the number of connected triplets of nodes in G.

31. Applying the Hadamard inequality (8.93) for the determinant of a matrix yields, with (2.2),

$$|\det A| \leq \prod_{j=1}^{N} \left(\sum_{i=1}^{N} a_{ji}^2 \right)^{\frac{1}{2}} = \prod_{j=1}^{N} \left(\sum_{i=1}^{N} a_{ji} \right)^{\frac{1}{2}} = \prod_{j=1}^{N} \sqrt{d_j}$$

Hence, with (8.6),

$$(\det A)^2 = \prod_{k=1}^{N} \lambda_k^2 \leq \prod_{j=1}^{N} d_j \tag{3.7}$$

32. Art. 158 relates the diagonal elements of a symmetric matrix to its eigenvalues. Since $a_{jj} = 0$, the matrix equation (8.35) becomes $Y\lambda = 0$, where the vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ and where the non negative matrix $Y^T = \begin{bmatrix} y_1 & y_2 & \cdots & y_N \end{bmatrix}$ consists of column vectors $y_j = \left(x_{1j}^2, x_{2j}^2, \ldots, x_{Nj}^2\right)$, where x_{kj} is the j th component of the k th eigenvector of A belonging to λ_k. Geometrically, $Y\lambda = 0$ means that the vector λ is orthogonal to all N vectors y_j and, in order to have a non zero solution for λ, there must hold that $\det Y = 0$. This means, that the matrix Y has a zero eigenvalue, while all other eigenvalues of Y lie, as shown in **art.** 158, within the unit circle and the largest eigenvalue is precisely equal to 1. In addition, $\det Y = 0$ implies that the set of vectors $y_1, y_2, \ldots, y_N$ is linearly dependent! Since the k th row of Y equals the vector z_k consisting of the squared components of the k th eigenvector x_k, the property $\det Y = \det Y^T = 0$ also implies that the vectors $z_1, z_2, \ldots, z_N$ are linearly dependent.

Since $\left(A^2\right)_{jj} = d_j$, another instance of (8.36) gives

$$Y^T \lambda^2 = d$$

where the vector $\lambda^2 = \left(\lambda_1^2, \lambda_2^2, \ldots, \lambda_N^2\right)$ and $d = (d_1, d_2, \ldots, d_N)$ is the degree vector. Since $Yu = u$ (**art.** 158), left multiplying with u yields $u^T \lambda^2 = 2L$, which is (3.5).

3.2 The number of walks

33. The total number N_k of walks of length k in a graph follows from Lemma 3 as

$$N_k = \sum_{i=1}^{N} \sum_{j=1}^{N} (A^k)_{ij} = u^T A^k u \tag{3.8}$$

For example, $N_0 = N$, $N_1 = 2L$. Invoking (2.4) and $A^T = A$, we can write

$$N_k = u^T A^T A^{k-2} A u = d^T A^{k-2} d$$

For example, if $k = 2$, we obtain $N_2 = d^T d$, or

$$N_2 = \sum_{k=1}^{N} d_k^2 = N \left((E\,[D])^2 + \mathrm{Var}\,[D] \right) \tag{3.9}$$

The number of walks $\{N_0, N_1, \ldots, N_{10}\}$ in the graph of Fig. 2.1 ignoring directions and up to $k = 10$ is $\{6, 18, 56, 174, 542, 1688, 5258, 16378, 51016, 158910, 494990\}$.

Since the adjacency matrix A is symmetric, **art.** 156 provides us with

$$A^k = \sum_{n=1}^{N} \lambda_n^k x_n x_n^T \tag{3.10}$$

such that total number $N_k = u^T A^k u$ of walks of length k is expressed in terms of

the eigenvalues of A as

$$N_k = \sum_{n=1}^{N} \left(x_n^T u\right)^2 \lambda_n^k \tag{3.11}$$

where $x_n^T u = \sum_{j=1}^{N} (x_n)_j$ is the sum of the components of the eigenvector x_n. When the (normalized) eigenvector $x_1 = \frac{u}{\sqrt{N}}$ as in regular graphs (**art.** 41) where $\lambda_1 = r$, the number of all walks with k hops equals $N_k = Nr^k$. Geometrically, the scalar product $x_n^T u = \sum_{j=1}^{N} (x_n)_j$ is the projection of the eigenvector x_n onto the vector u,

$$x_n^T u = \|x_n\|_2 \|u\|_2 \cos \alpha_n = \sqrt{N} \cos \alpha_n \tag{3.12}$$

where α_n is the angle between the eigenvector x_n and the all one vector u. The total number N_k of walks of length k, written in terms of the "graph angles" as coined by Cvetković *et al.* (1997), is

$$N_k = N \sum_{n=1}^{N} \lambda_n^k \cos^2 \alpha_n \tag{3.13}$$

Since $N_k = u^T A^m A^{k-m} u = (A^m u)^T \left(A^{k-m} u\right)$, the Cauchy Schwarz inequality (8.41) shows that

$$\left| (A^m u)^T \left(A^{k-m} u\right) \right|^2 \le \left((A^m u)^T (A^m u) \right) \left(\left(A^{k-m} u\right)^T \left(A^{k-m} u\right) \right)$$

from which we obtain, for integers $k \ge 0$, the inequality

$$N_k^2 \le \left(u^T A^{2m} u\right) \left(u^T A^{2(k-m)} u\right) \tag{3.14}$$

valid for any number m, provided A^m exists and A^m is a real matrix. Equality only holds for regular graphs. If $2m$ is an integer, we have $N_k^2 \le N_{2m} N_{2k-2m}$. In particular for $m = 0$, there holds that $N_k^2 \le N N_{2k}$. When $2m = 1$, we would erroneously deduce that $N_k^2 \le (2L) N_{2k-1}$, which is wrong because $A^{1/2} = X^T \text{diag}\left(\sqrt{\lambda_k (A)}\right) X$ is a not a real matrix (as is required for the application of the Cauchy Schwarz inequality), because at least one eigenvalue $\lambda_N (A)$ is negative.

34. *The generating function $N_G (z)$.* The generating function of the total number of walks in a graph G is defined as

$$N_G (z) = \sum_{k=0}^{\infty} N_k z^k \tag{3.15}$$

The two different expressions in **art.** 33 result in two different expressions for $N_G (z)$. First, substituting the definition (3.8) into (3.15) yields

$$N_G (z) = u^T \left(\sum_{k=0}^{\infty} A^k z^k \right) u = u^T (I - zA)^{-1} u \tag{3.16}$$

where $|z| < \frac{1}{\lambda_1}$ in order for the infinite series to convergence (**art.** 149). Since A is symmetric, there holds for any analytic function $f(z)$ (possessing a power series expansion around some point) that $f(A) = (f(A))^T$. Thus, we have that

$$u^T (I - zA)^{-1} u = u^T \left((I - zA)^{-\frac{1}{2}} \right)^T (I - zA)^{-\frac{1}{2}} u = \left\| (I - zA)^{-\frac{1}{2}} u \right\|_2^2$$

which shows that

$$N_G(z) = \left\| (I - zA)^{-\frac{1}{2}} u \right\|_2^2 \geq 0$$

for all real z obeying $|z| < \frac{1}{\lambda_1}$. The zeros of $N_G(z)$ are simple and lie in between two consecutive eigenvalues of A as follows from **art.** 180.

Second, invoking (3.11) gives, for $|z| < \frac{1}{\lambda_1}$,

$$N_G(z) = \sum_{n=1}^{N} \left(x_n^T u \right)^2 \sum_{k=0}^{\infty} \lambda_n^k z^k = \sum_{n=1}^{N} \frac{\left(x_n^T u \right)^2}{1 - \lambda_n z} \tag{3.17}$$

Since $N_G(0) = N_0 = N$, we have

$$N = \sum_{n=1}^{N} \left(x_n^T u \right)^2 \tag{3.18}$$

and, with (3.13),

$$\sum_{n=1}^{N} \cos^2 \alpha_n = 1$$

For regular graphs (**art.** 41), where $x_1 = \frac{u}{\sqrt{N}}$ is the eigenvector belonging to $\lambda_1 = r$, the generating function (3.17) of the total number of walks simplifies to

$$N_{\text{regular graph}}(z) = \frac{N}{1 - rz} \tag{3.19}$$

Cvetković *et al.* (1995, p. 45) have found an elegant formula for $N_G(z)$ by rewriting $u^T (I - zA)^{-1} u$ using (8.81). Indeed, for $k = 1$ in (8.81) and $C_{N \times 1} = xu$ and $D_{N \times 1} = u$, we obtain with $J = u.u^T$,

$$\det (A + zJ) = \det A \det \left(1 + zu^T A^{-1} u \right) = \left(1 + zu^T A^{-1} u \right) \det A$$

Replacing $A \to I - zA$ results in

$$u^T (I - zA)^{-1} u = \frac{1}{z} \left(\frac{\det (I + z (J - A))}{\det (I - zA)} - 1 \right)$$

The right hand side can be written in terms of the complement $A^c = J - I - A$ as

$$u^T (I - zA)^{-1} u = \frac{1}{z} \left((-1)^N \frac{\det \left(A^c + \frac{z+1}{z} I \right)}{\det \left(A - \frac{1}{z} I \right)} - 1 \right)$$

Finally, using the characteristic polynomial of a matrix A, $c_A(z) = \det(A - zI)$, we arrive at Cvetkovic's formula, for $|z| < \frac{1}{\lambda_1}$,

$$N_G(z) = \frac{1}{z}\left((-1)^N \frac{c_{A^c}\left(-\frac{1}{z} - 1\right)}{c_A\left(\frac{1}{z}\right)} - 1\right) \tag{3.20}$$

which shows that $zN_G(z) + 1$ is a ratio of two real polynomials, both with real zeros and of degree at most N.

The right hand side of (3.16), (3.17) and (3.20) can serve as analytic continuations of $N_G(z)$ for $|z| \geq \frac{1}{\lambda_1}$.

35. *The total number of walks N_k and the sum of degree powers.* We will prove the inequality

$$N_k \leq \sum_{j=1}^{N} d_j^k \tag{3.21}$$

due to Fiol and Garriga (2009). Equality in (3.21) for all $k \geq 0$ is only achieved for regular graphs, because $N_{k;\text{regular graph}} = Nr^k$ (**art. 33**). For $k \leq 2$, equality in (3.21) holds in general, because $N_0 = N = \sum_{j=1}^{N} d_j^0$, $N_1 = 2L = \sum_{j=1}^{N} d_j$ and $N_2 = d^T d = \sum_{j=1}^{N} d_j^2$. For $k > 2$, the total number N_k of walks of length k is

$$N_k = u^T A^T A^{k-2} A u = d^T A^{k-2} d = \sum_{i=1}^{N}\sum_{j=1}^{N} d_i \left(A^{k-2}\right)_{ij} d_j$$

$$= \sum_{i=1}^{N} \left(A^{k-2}\right)_{ii} d_i^2 + 2\sum_{i=1}^{N}\sum_{j=i+1}^{N} d_i \left(A^{k-2}\right)_{ij} d_j$$

where the last sum holds by symmetry of $A = A^T$. From $0 \leq (a-b)^2 = a^2 + b^2 - 2ab$, we see that $a^2 + b^2 \geq 2ab$ such that

$$2\sum_{i=1}^{N}\sum_{j=i+1}^{N} d_i \left(A^{k-2}\right)_{ij} d_j \leq \sum_{i=1}^{N}\sum_{j=i+1}^{N} \left(A^{k-2}\right)_{ij} \{d_i^2 + d_j^2\}$$

and

$$N_k \leq \sum_{i=1}^{N} \left(A^{k-2}\right)_{ii} d_i^2 + \sum_{i=1}^{N}\sum_{j=i+1}^{N} \left(A^{k-2}\right)_{ij} \{d_i^2 + d_j^2\} = \sum_{i=1}^{N}\sum_{j=1}^{N} \left(A^{k-2}\right)_{ij} d_j^2$$

$$= u^T A^{k-2} d^2$$

where the vector $d^j = \left(d_1^j, d_2^j, \ldots, d_N^j\right)$. This derivation suggests the induction argument

$$N_k \leq u^T A^{k-m} d^m \leq u^T A^{k-m-1} d^{m+1} \tag{3.22}$$

which has been demonstrated already for $m = 0, 1$ and 2. Assume now that it holds

for $m = \nu \geq 0$, then the induction inequality (3.22) is proved when we can show that it also holds for $m = \nu + 1$. Using $Au = d$ in (2.4) and $A = A^T$,

$$u^T A^{k-\nu} d^\nu = u^T A^T A^{k-\nu-1} d^\nu = d^T A^{k-\nu-1} d^\nu = \sum_{i=1}^{N}\sum_{j=1}^{N} d_i \left(A^{k-\nu-1}\right)_{ij} d_j^\nu$$

$$= \sum_{i=1}^{N}\left(A^{k-\nu-1}\right)_{ij} d_i^{\nu+1} + \sum_{i=1}^{N}\sum_{j=i+1}^{N}\left(A^{k-\nu-1}\right)_{ij}\left(d_i d_j^\nu + d_j d_i^\nu\right)$$

Fiol and Garriga (2009) now cleverly use the inequality for any positive numbers a and b,

$$a^k b + a b^k = a^{k+1} + b^{k+1} - \left(a^k - b^k\right)(a - b) \leq a^{k+1} + b^{k+1}$$

with equality if and only if $a = b$, and obtain

$$u^T A^{k-\nu} d^\nu \leq \sum_{i=1}^{N}\left(A^{k-\nu-1}\right)_{ij} d_i^{\nu+1} + \sum_{i=1}^{N}\sum_{j=i+1}^{N}\left(A^{k-\nu-1}\right)_{ij}\left(d_j^{\nu+1} + d_i^{\nu+1}\right)$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\left(A^{k-\nu-1}\right)_{ij} d_j^{\nu+1} = u^T A^{k-(\nu+1)} d^{\nu+1}$$

which establishes the induction inequality (3.22) and completes the proof of (3.21).

By using the fundamental form of the Laplacian (4.11) in **art. 77**, applied to $x = d$,

$$d^T Q d = \sum_{l \in \mathcal{L}} \left(d_{l+} - d_{l-}\right)^2$$

and $d^T Q d = d^T (\Delta - A) d = \sum_{j=1}^{N} d_j^3 - d^T A d$, we find that

$$\sum_{j=1}^{N} d_j^3 - N_3 = \sum_{l \in \mathcal{L}} \left(d_{l+} - d_{l-}\right)^2 = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(d_i - d_j\right)^2 a_{ij} \tag{3.23}$$

where the right hand side sums, over all links l in the graph, the square of the difference between the degrees at both side of the link l. We will see in Section 7.5 how this expression can be related to the linear correlation coefficient of the degrees in a graph and to the (dis)assortative property of a graph.

36. The number of closed walks W_k of length k in graph G is defined in **art. 17**; Lemma 3 and **art. 144** show that

$$W_k = \sum_{j=1}^{N}(A^k)_{jj} = \text{trace}\left(A^k\right) = \sum_{j=1}^{N}\lambda_j^k \tag{3.24}$$

Since the mean $E[\lambda] = 0$ (**art. 25**), the definition (3.24) demonstrates that all centered moments of the adjacency eigenvalues are non negative and equal to

$$E\left[(\lambda - E[\lambda])^k\right] = \frac{W_k}{N}$$

Hence, the centered k th moment is equal to the number of a closed walks of length k per node. The special case for $k = 2$ is $\text{Var}[\lambda] = \frac{2L}{N}$, which is deduced in **art. 27**. When $k = 3$, (3.3) indicates that

$$E\left[(\lambda - E[\lambda])^3\right] = \frac{6\blacktriangle_G}{N}$$

The skewness s_λ, that measures the lack of symmetry of the distribution around the mean, is defined as the normalized third moment,

$$s_\lambda = \frac{E\left[(\lambda - E[\lambda])^3\right]}{\left(E\left[(\lambda - E[\lambda])^2\right]\right)^{3/2}} = \frac{3\blacktriangle_G}{L\sqrt{E[D]}}$$

Since a tree does not have triangles, $\blacktriangle_G = 0$, the minimum possible skewness, $s_\lambda = 0$, in the distribution of adjacency eigenvalues is achieved for a tree. In Section 5.8, we will indeed show that only the adjacency spectrum of a tree is symmetric around the mean (or origin $\lambda = 0$).

The number of closed walks W_k of length k in graph G has a nice generating function, which is derived from Jacobi's general identity (**art. 193**). Let $C = zA$ in (8.89),

$$\text{trace}\log(I - zA) = \log\det(I - zA)$$

and expand

$$\log(I - zA) = \sum_{k=1}^{\infty} \frac{(zA)^k}{k}$$

This Taylor series converges (**art. 149**) provided $|z| < \frac{1}{\lambda_1}$. After differentiation with respect to z, we obtain

$$\frac{1}{z}\sum_{k=1}^{\infty} \text{trace}\left(A^k\right) z^k = \frac{d}{dz}\log\det(I - zA)$$

With $W_k = \text{trace}(A^k)$ and $W_0 = N$, the generating function of the number of closed walks W_k in G and convergent for $|z| < \frac{1}{\lambda_1}$ is

$$W_G(z) = \sum_{k=0}^{\infty} W_k z^k = N + z\frac{d}{dz}\log\det(I - zA) \qquad (3.25)$$

Substitution of the last equality in (3.24) into the generating function (3.25) yields, for $|z| < \frac{1}{\lambda_1}$,

$$W_G(z) = \sum_{j=1}^{N}\sum_{k=0}^{\infty} \lambda_j^k z^k = \sum_{j=1}^{N} \frac{1}{1 - \lambda_j z} \qquad (3.26)$$

In terms of the characteristic polynomial $c_A(\lambda) = \sum_{k=0}^{N} c_k \lambda^k$ of A, which is

$c_A(\lambda) = \det(A - \lambda I) = (-\lambda)^N \det\left(I - \frac{1}{\lambda}A\right)$, we have

$$\det(I - zA) = (-z)^N c_A(z^{-1}) = \sum_{k=0}^{N} (-1)^N c_{N-k} z^k$$

with $(-1)^N c_N = 1$. Then, we deduce from (3.25) that

$$\sum_{k=0}^{N} (-1)^N c_{N-k} z^k = \exp\left(\sum_{k=1}^{\infty} W_k \frac{z^k}{k}\right)$$

from which, by Taylor's theorem,

$$(-1)^N c_{N-k} = \frac{1}{k!} \frac{d^k}{dz^k} \exp\left(\sum_{k=1}^{\infty} \frac{W_k}{k} z^k\right)\Bigg|_{z=0}$$

This relation is equivalent to the Newton identities (**art. 26**). In fact, by applying our characteristic coefficients defined in Van Mieghem (2007), the above derivatives can be explicitly computed for any finite k. The result leads precisely to that in **art. 26**.

37. The generating function of the number of closed walks of length k that start and terminate at node j (**art. 17**), is defined as

$$W_G(z; j) = \sum_{k=0}^{\infty} \left(A^k\right)_{jj} z^k \tag{3.27}$$

Substituting the j th diagonal element of (3.10) into (3.27) yields, for $|z| < \frac{1}{\lambda_1}$,

$$W_G(z; j) = \sum_{n=1}^{N} \left(x_n x_n^T\right)_{jj} \sum_{k=0}^{\infty} \lambda_n^k z^k = \sum_{n=1}^{N} \frac{\left(x_n x_n^T\right)_{jj}}{1 - \lambda_n z}$$

Art. 157 indicates that $\left(x_k x_k^T\right)_{jj} = \left((x_k)_j\right)^2$, such that

$$W_G(z; j) = \sum_{n=1}^{N} \frac{\left((x_n)_j\right)^2}{1 - \lambda_n z} \tag{3.28}$$

Clearly, by definition, we have that $W_G(z) = \sum_{j=1}^{N} W_G(z; j)$, while (3.26) and (3.28) indicate that $\sum_{j=1}^{N} \left((x_n)_j\right)^2 = 1$, which confirms the normalization $x_n^T x_n = 1$ of the eigenvector x_n.

Combining (8.65) and (8.66) in **art. 178** yields

$$\frac{\det\left(zI - A_{\backslash\{j\}}\right)}{\det(zI - A)} = \sum_{n=1}^{N} \frac{\left(x_n x_n^T\right)_{jj}}{z - \lambda_n}$$

where $A_{\backslash\{j\}}$ is the $(N-1) \times (N-1)$ adjacency matrix obtained from A by deleting the j th row and column. Thus, $A_{\backslash\{j\}}$ is the adjacency matrix of the subgraph

$G \setminus \{j\}$ of G obtained from the graph G by deleting node j and all its incident links. Hence,

$$\frac{\det \left(zI - A_{\setminus \{j\}}\right)}{\det \left(zI - A\right)} = \frac{1}{z} W_G \left(\frac{1}{z}; j\right)$$

and written in terms of the characteristic polynomial of a matrix A, $c_A(z) = \det(A - zI)$, we obtain

$$W_G(z; j) = -\frac{c_{A_{\setminus \{j\}}} \left(\frac{1}{z}\right)}{z c_A \left(\frac{1}{z}\right)}$$

The relation between the characteristic polynomials $c_{A_{\setminus \{j\}}}(z)$ and $c_A(z)$ is further studied in **art.** 60.

38. *Relations between N_k and W_k.* Let m be the maximizer of $x_k^T u$ over all $1 \leq k \leq N$ eigenvectors such that $x_m^T u \geq x_k^T u$ for any $1 \leq k \neq m \leq N$. Geo metrically, the "graph angle" representation in (3.12), $x_k^T \frac{u}{\sqrt{N}} = \cos(\alpha_k)$, reflects that all orthogonal eigenvectors $x_1, x_2, \ldots, x_N$ start at the origin and end on an N dimensional unit sphere centered at the origin. The graph angle between x_k and $\frac{u}{\sqrt{N}}$ is largest for x_1, by the Perron Frobenius Theorem 38 in **art.** 168, because x_1 and $\frac{u}{\sqrt{N}}$ lie in the same N dimensional "quadrant" as both their components are non negative. Any other vector x_k must be orthogonal to x_1, implying that x_k cannot lie in the "opposite" N dimensional "quadrant", where all components or coordinates are negative, and in which the resulting $\cos(\alpha_k)$ also can be large. An other, though less transparent, argument follows from the Cauchy identity (8.86),

$$\left(u^T x_k\right)^2 = N - \frac{1}{2} \sum_{j=1}^{N} \sum_{l=1}^{N} \left((x_k)_j - (x_k)_l\right)^2$$

$$= N - \sum_{j=1}^{N} \sum_{l=1}^{j} \left((x_k)_j - (x_k)_l\right)^2$$

which illustrates that the maximizer over all $\left(u^T x_k\right)^2$ has minimum difference be tween its components. Thus, it is the eigenvector x_m that is as close as possible to the vector $\frac{1}{\sqrt{N}} u$ with all components exactly the same. In conclusion, $m = 1$ and $x_1^T u > x_k^T u$ for all $1 < k \leq N$. **Art.** 162 further demonstrates that $x_1^T u \geq 1$, because $x_1^T u = \sum_{j=1}^{N} (x_1)_j = \sum_{j=1}^{N} \left|(x_1)_j\right| = \|x_1\|_1$ and $\|x_1\|_1 \geq \|x_1\|_2 = 1$.

Likewise, let q be the index that minimizes $\left(x_k^T u\right)^2 \geq \left(x_q^T u\right)^2$ for any $1 \leq k \neq q \leq N$. Recall that $x_q^T u = 0$ for a regular graph. Then, (3.11) is lower and upper bounded as

$$\left(x_q^T u\right)^2 \sum_{n=1}^{N} \lambda_n^k \leq \sum_{n=1}^{N} \left(x_n^T u\right)^2 \lambda_n^k \leq \left(x_1^T u\right)^2 \sum_{n=1}^{N} \lambda_n^k$$

Invoking the number of closed walks W_k of length k in graph G (**art.** 36), $W_k =$

$\sum_{n=1}^{N} \lambda_n^k$, and the total number N_k of walks (3.11), leads to the inequality

$$\left(x_q^T u\right)^2 W_k \leq N_k \leq \left(x_1^T u\right)^2 W_k < N W_k$$

where the last inequality follows from (3.18).

The $N \times 1$ total walk vector $\mathbf{N} = (N, N_1, N_2, \ldots, N_{N-1})$ can be written with (3.11) as

$$
\begin{bmatrix}
N \\
N_1 \\
\vdots \\
N_{N-2} \\
N_{N-1}
\end{bmatrix}
=
\begin{bmatrix}
1 & 1 & \cdots & 1 & 1 \\
\lambda_1 & \lambda_2 & \vdots & \lambda_{N-1} & \lambda_N \\
\vdots & \vdots & \cdots & \vdots & \vdots \\
\lambda_1^{N-2} & \lambda_2^{N-2} & \cdots & \lambda_{N-1}^{N-2} & \lambda_N^{N-2} \\
\lambda_1^{N-1} & \lambda_2^{N-1} & \cdots & \lambda_{N-1}^{N-1} & \lambda_N^{N-1}
\end{bmatrix}
\cdot
\begin{bmatrix}
\left(u^T x_1\right)^2 \\
\left(u^T x_2\right)^2 \\
\vdots \\
\left(u^T x_{N-1}\right)^2 \\
\left(u^T x_N\right)^2
\end{bmatrix}
$$

and, in matrix notation,

$$\mathbf{N} = V_N\left(\lambda\right) t_x$$

where $V_N\left(\lambda\right)$ is the Vandermonde matrix (8.90) in **art.** 194 and where the $N \times 1$ vector t_x has $\left(u^T x_k\right)^2$ as its k th component. Similarly, the closed walk vector $\mathbf{W} = (W_0, W_1, W_2, \ldots, W_{N-1})$ is written as

$$\mathbf{W} = V_N\left(\lambda\right) u$$

39. *Diameter of a graph.*

Theorem 5 *The number of distinct eigenvalues of the adjacency matrix A is at least equal to $\rho + 1$, where ρ is the diameter of the graph.*

First proof: Lemma 3 implies that $\left(A^k\right)_{ij}$ is non zero if and only if node i and j can be joined in the graph by a walk of length k. Thus, if the shortest path from node i to j consists of h hops, then $\left(A^h\right)_{ij} \neq 0$, while $\left(A^k\right)_{ij} = 0$ if $k < h$. This means that the matrix A^h cannot be written as a linear combination of $I, A, A^2, \ldots, A^{h-1}$. By definition of the diameter ρ as the longest shortest path, we thus conclude that the matrices $I, A, A^2, \ldots, A^\rho$ are linearly independent. **Art.** 156 shows that the matrix E_k, that represents the orthogonal projection onto the eigenspace of λ_k, is a polynomial in A. Thus, the vector space spanned by $I, A, A^2, \ldots, A^\rho$ is also spanned by a corresponding set of matrices E_k, which obey $E_k E_m = 1_{\{k=m\}}$ (**art.** 156). Let $Y = \sum_{k=1}^{\rho+1} c_k E_k$, then $c_j = E_j Y$, which is only zero if all E_k are linearly independent. The matrices E_k and E_m are only linearly independent if they belong to a distinct eigenvalue of A. The linear independence of the set $I, A, A^2, \ldots, A^\rho$ thus implies that at least $\rho + 1$ eigenvalues of A must be distinct. $\qquad \square$

We may rephrase Theorem 5 as: "The diameter ρ of a graph G obeys $\rho \leq l - 1$, where l is the number of different eigenvalues of A". The second proof may be found easier and more elegant.

Second proof: As defined in **art.** 19, the lowest integer ρ, which satisfies $(A^\rho)_{ij} \neq 0$ and $(A^m)_{ij} = 0$ if $m < \rho$ for each pair (i, j) of nodes, is called the *diameter* of the graph G. Suppose that the adjacency matrix A has precisely l distinct eigenvalues. **Art.** 145 shows that A obeys $m_{c_A}(A) = O$, where the minimal polynomial $m_{c_A}(x) = \sum_{k=0}^l b_k z^k$ has degree l. Hence, we may write

$$\left(A^l\right)_{ij} = -\frac{1}{b_l} \sum_{k=0}^{l-1} b_k \left(A^k\right)_{ij}$$

which shows that $\rho \leq l - 1$. For, assume that $\rho > l - 1$, then there is at least one pair (i, j) for which $\left(A^k\right)_{ij} = 0$ for $0 \leq k \leq l-1$. But, the minimal polynomial then shows that also $\left(A^l\right)_{ij} = 0$ and, further any $\left(A^{l+q}\right)_{ij} = 0$ because $A^q m_{c_A}(A) = O$ for any integer $q \geq 0$. This leads to a contradiction that $\rho > l - 1$. $\qquad\square$

As an example, consider the complete graph K_N whose adjacency matrix has precisely $l = 2$ distinct eigenvalues, $\lambda_1 = N - 1$ and $\lambda_2 = -1$, as computed in Section 5.1. Theorem 5 states that the diameter is at most $\rho = l - 1 = 1$. Since the diameter is at least equal to $\rho = 1$, we conclude from Theorem 5 that the diameter in the complete graph equals $\rho = 1$, as anticipated.

40. The characteristic polynomial of the complement G^c is

$$
\begin{aligned}
\det\left(A^c - \lambda I\right) &= \det\left(J - A - (\lambda + 1) I\right) \\
&= (-1)^N \det\left((A + (\lambda + 1) I)\left(I - (A + (\lambda + 1) I)^{-1} J\right)\right) \\
&= (-1)^N \det\left((A + (\lambda + 1) I)\right) \det\left(I - (A + (\lambda + 1) I)^{-1} u.u^T\right)
\end{aligned}
$$

where we have used that $J = u.u^T$. Using the "rank 1 update" formula (8.82), we find

$$\det\left(A^c - \lambda I\right) = (-1)^N g(\lambda) \det\left(A + (\lambda + 1) I\right) \qquad (3.29)$$

with the definition

$$
\begin{aligned}
g(\lambda) &= 1 - u^T \left(A + (\lambda + 1) I\right)^{-1} u \\
&= 1 + z N_G(z)\big|_{z = \frac{1}{\lambda+1}}
\end{aligned}
$$

where the last equation is written in terms of the generating function (3.16) of the total number of walks (**art.** 34). In general, $g(\lambda)$ is not a simple function of λ although a little more is known. For example, $g(\lambda) = 1 - \left\|\left(A + (\lambda + 1) I\right)^{-\frac{1}{2}} u\right\|_2^2$, which shows that $g(\lambda) \in (-\infty, 1]$. Analogous to derivations in **art.** 34, we can express $g(\lambda)$ in terms of "graph angles" as

$$g(\lambda) = 1 - N \sum_{j=1}^N \frac{\cos^2 \alpha_j}{\lambda + 1 + \lambda_j}$$

which shows that the largest zero of $g(\lambda)$ lies on the positive real λ axis exceeding $-\lambda_N - 1$. In Section 5.9, we give two methods to approximate this largest zero arbitrarily close. With (8.5), we have $c_A(-\lambda - 1) = \det(A + (\lambda + 1)I) = \prod_{k=1}^{N}(\lambda_k + 1 + \lambda)$. Thus, the characteristic polynomial $c_{A^c}(\lambda)$ of the complement A^c is

$$\det(A^c - \lambda I) = \frac{(-1)^N}{N} \sum_{j=1}^{N} \left(\lambda + 1 + \lambda_j - N^2 \cos^2 \alpha_j\right) \prod_{k=1;k\neq j}^{N}(\lambda_k + 1 + \lambda) \quad (3.30)$$

which shows that the poles of $g(\lambda)$ are precisely compensated by the zeros of the characteristic polynomial $c_A(-\lambda - 1)$. Thus, the eigenvalues of A^c are generally different from $\{-\lambda_j - 1\}_{1 \leq j \leq N}$, where λ_j is an eigenvalue of A. Only if u is an eigenvector of A corresponding with λ_k, then $g(\lambda) = \frac{\lambda + 1 + \lambda_k}{\lambda + 1 + \lambda_k} N$ and all eigenvalues of A^c belong to the set $\{-\lambda_j - 1\}_{1 \leq j \neq k \leq N} \cup \{N - 1 - \lambda_k\}$. According to **art. 41**, u can only be an eigenvector belonging to λ_1 when the graph is regular.

Combining (3.17) and (3.20) yields, with $\lambda = \frac{1}{z}$,

$$(-1)^N \frac{c_{A^c}(-\lambda - 1)}{c_A(\lambda)} = 1 + \sum_{n=1}^{N} \frac{\left(x_n^T u\right)^2}{\lambda - \lambda_n}$$

The right hand side can be written as a fraction of two polynomials, in which the denominator polynomial has only simple zeros. From this observation, Cvetković *et al.* (1995) deduced that, if $c_A(\lambda)$ has an eigenvalue λ with multiplicity $p > 1$, then the characteristic polynomial of the complement $c_{A^c}(\lambda)$ contains an eigenvalue $-\lambda - 1$ with multiplicity $p - 1 \leq q \leq p + 1$.

3.3 Regular graphs

The class of regular graph possesses a lot of specific and remarkable properties that justify the discussion of some spectrum related properties here.

41. *Regular graphs.* Every node j in a regular graph has the same degree $d_j = r$ and relation (2.2) indicates that each row sum of A equals r. The basic law of the degree (2.3) reduces for regular graphs to $2L = Nr$, implying that, if the degree r is odd, then the number of nodes N must be even.

Theorem 6 *The maximum degree $d_{\max} = \max_{1 \leq j \leq N} d_j$ is the largest eigenvalue of the adjacency matrix A of a connected graph G if and only if the corresponding graph is regular (i.e., $d_j = d_{\max} = r$ for all j).*

Proof: If x is an eigenvector of A belonging to eigenvalue $\lambda = d_{\max}$ so is each vector kx for each complex k (**art. 138**). Thus, we can scale the eigenvector x such that the maximum component, say $x_m = 1$, and $x_k \leq 1$ for all k. The eigenvalue

equation $Ax = d_{\max}x$ for that maximum component x_m is

$$d_{\max}x_m = d_{\max} = \sum_{j=1}^{N} a_{mj}x_j$$

which implies that all $x_j = 1$ whenever $a_{mj} = 1$, i.e., when the node j is adjacent to node m. Hence, the degree of node m is $d_m = d_{\max}$. For any node j adjacent to m for which the component $x_j = 1$, a same eigenvalue relation holds and thus $d_j = d_{\max}$. Proceeding with this process shows that every node $k \in G$ has same degree $d_k = d_{\max}$ because G is connected. Hence, $x = u$ where $u^T = [1 \ 1 \ \cdots \ 1]$ and the Perron Frobenius Theorem 38 shows that u is the eigenvector belonging to the largest eigenvalue of A. Conversely, if G is connected and regular, then $\sum_{j=1}^{N} a_{mj} = d_{\max} = r$ for each m such that u is the eigenvector belonging to eigenvalue $\lambda = d_{\max}$, and the only possible eigenvector (**art.** 21). Hence, there is only one eigenvalue $d_{\max} = r$. □

Theorem 6 shows that, for a regular graph, $Au = ru$, and, thus, $AJ = rJ$. After taking the transpose, $(AJ)^T = JA = rJ$, we see that $AJ = JA$. Thus, A and J commute if G is regular.

Theorem 7 (Hoffman) *A graph G is regular and connected if and only if there exists a polynomial p such that $J = p(A)$.*

Proof: (a) If $J = p(A)$, then J and A commute and, hence, G is regular. (b) Since the largest eigenvalue r is simple (**art.** 21), the Laplacian $Q = rI - A$ has a zero eigenvalue with multiplicity 1. Theorem 11 then states that a regular graph G is connected. Conversely, let G be connected and regular. We can diagonalize the adjacency matrix A of G by using an orthogonal matrix formed by its eigenvectors (**art.** 151). This basis of eigenvectors of A also diagonalizes J as $\mathrm{diag}(N, 0, \ldots, 0)$, because J and A commute. Consider the polynomial

$$q(x) = \frac{c_A(x)}{x - r} = \prod_{j=2}^{N} (\lambda_k(A) - x)$$

where $c_A(x)$ is the characteristic polynomial of A, then $J = N\frac{q(A)}{q(r)}$, because the projections on the basisvectors are $q(A)x_j = 0$ if $x_j \neq u$ and $q(A)u = q(r)u$, while $Ju = Nu$. Thus, the polynomial $p(x) = N\frac{q(x)}{q(r)}$ satisfies the requirement. □

The proof shows that, if $m_{c_A}(x)$ is the minimal polynomial (**art.** 145) associated to the characteristic polynomial $c_A(x)$ and $q_{m_c}(x) = \frac{m_{c_A}(x)}{x \ r}$, the polynomial $p_{m_c}(x) = N\frac{q_{m_c}(x)}{q_{m_c}(r)}$ of possibly lower degree can be found.

42. *Strongly regular graphs.* Following Cvetković *et al.* (1995), we first define $\varpi(v, w)$ as the number of nodes adjacent to *both* node v and node $w \neq v$. In other words, $\varpi(v, w)$ is the number of common neighbors of both v and w. A regular graph G of degree $r > 0$, different from the complete graph K_N, is called strongly

regular if $\varpi(v,w) = n_1$ for each pair (v,w) of adjacent nodes and $\varpi(v,w) = n_2$ for each pair (v,w) of non adjacent nodes.

A strongly regular graph is completely defined by the parameters (N, r, n_1, n_2). For example, the Petersen graph in Fig. 2.3 is a strongly regular graph with para meters $(10, 3, 0, 1)$. Cvetković *et al.* (2009) show how many strongly regular graphs can be constructed from line graphs. For example, the line graph $l(K_N)$ of the complete graph is strongly regular with parameters $\left(\frac{N(N-1)}{2}, 2N-4, N-2, 4\right)$ for $N > 3$. Another example is the class of Paley graphs P_q, whose nodes belong to the finite field $\mathbb{F}_q$ of order q, where q is a prime power congruent to 1 modulo 4, and whose links (i, j) are present if and only if $i - j$ is a quadratic residue (see Hardy and Wright (1968)). The Paley graph P_q is strongly regular with parame ters $\left(|\mathbb{F}_q|, \frac{q-1}{2}, \frac{q-5}{4}, \frac{q-1}{4}\right)$. Bollobas (2001, Chapter 13) discusses properties of the Paley graph and its generalizations, the Caley graphs and conference graphs.

The number of common neighbors of two different nodes i and j is equal to the number of 2 hop walks between i and j. Thus, Lemma 3 states that $\varpi(i, j) = \left(A^2\right)_{ij}$ if $i \neq j$. **Art.** 30 shows that $\left(A^2\right)_{ii} = d_i = r$. The condition for strong regularity states that, for different nodes i and j, $\left(A^2\right)_{ij} = n_1 a_{ij} + n_2(1 - a_{ij})$, because $\varpi(i, j) = n_1$ if node i and j are neighbors, hence, $a_{ij} = 1$ and $\varpi(i, j) = n_2$, if they are not, i.e. $a_{ij} = 0$. Adding the two mutual exclusive conditions together with $\varpi(i, j) = \left(A^2\right)_{ij}$ demonstrates the relation. Combining all entries into a matrix form yields

$$A^2 = n_1 A + n_2 A^c + rI$$

Finally, using $A^c = J - I - A$ (**art.** 1), we obtain the matrix relation that charac terizes strong regularity,

$$A^2 = (n_1 - n_2) A + n_2 J + (r - n_2) I$$

from which $J = \frac{1}{n_2}\left(A^2 + (n_2 - n_1) A + (n_2 - r) I\right)$. Hence, the polynomial $J = p(A)$ in Hoffmans Theorem 7 is the quadratic polynomial

$$p_2(z) = \frac{1}{n_2}\left(z^2 + (n_2 - n_1) z + (n_2 - r)\right)$$

from which we deduce that the minimal polynomial $m_{c_A}(x) = \frac{q_{m_c}(r)}{N}(x - r) p_2(x)$ is of degree 3. The definition of a minimal polynomial in **art.** 211 implies that the adjacency matrix A of G possesses precisely three distinct eigenvalues $\lambda_1 = r$, λ_2 and λ_3, where λ_2 and λ_3 are zeros of $p_2(x)$, related by $n_1 - n_2 = \lambda_2 + \lambda_3$ and $n_2 - r = \lambda_2 \lambda_3$. The property that strongly regular graphs have three different eigenvalues explains why the complete graph K_N must be excluded in the definition above. In summary, we have proved:

Theorem 8 *A connected graph G is strongly regular with degree $r > 0$ if and only if its adjacency matrix A has three distinct eigenvalues $\lambda_1 = r$, λ_2 and λ_3, which*

satisfy

$$n_1 = r + \lambda_2 + \lambda_3 + \lambda_2\lambda_3$$
$$n_2 = r + \lambda_2\lambda_3$$

where n_1 and n_2 are the number of common neighbors of adjacent and non adjacent nodes, respectively.

3.4 Bounds for the largest, positive eigenvalue λ_1

The largest eigenvalue λ_1 of the adjacency matrix A appears in many applica tions. In particular in dynamic processes on graphs, the inverse of the largest eigen value λ_1 characterizes the threshold of the phase transition of both virus spread (Van Mieghem *et al.*, 2009) and synchronization of coupled oscillators (Restrepo *et al.*, 2005) in networks. Sharp bounds or exact expressions for λ_1 are desirable to control these processes. Bounds for λ_2 and λ_N in connected graphs follow from the general bounds (8.56) and (8.57), respectively, on eigenvalues of non negative, irreducible, symmetric matrices in **art.** 172.

43. *Classical lower bound.* The Rayleigh's inequalities in **art.** 152 indicate that

$$\lambda_1 = \sup_{x \neq 0} \frac{x^T A x}{x^T x}$$

and that the maximum is attained if and only if x is the eigenvector of A belonging to λ_1, while for any other vector $y \neq x$, $\lambda_1 \geq \frac{y^T A y}{y^T y}$. By choosing the vector $y = u$, we obtain, with (2.5), the classical bound

$$\lambda_1 \geq \frac{u^T A u}{u^T u} = \frac{2L}{N} \tag{3.31}$$

Equality is reached in a regular graph, because the average degree is $E[D] = \frac{2L}{N} = r$ since $d_j = r$ for each node j and, because r is the largest eigenvalue of A belonging to the eigenvector u (Theorem 6). The differences $\lambda_1 - E[D]$ and $d_{\max} - \lambda_1$ can be considered as measures for the irregularity of a graph.

The Interlacing Theorem 42 states that λ_1 is larger than or equal to the largest eigenvalue of any subgraph G_s of G:

$$\lambda_1 \geq \max_{\text{all } G_s \subset G} (\lambda_1(A_{G_s})) \tag{3.32}$$

Of course, the lower bounds deduced in this Section 3.4, such as (3.31) and (3.34), also apply to each individual subgraph G_s. It is a matter of ingenuity to find that subgraph G_s with highest largest eigenvalue $\lambda_1(A_{G_s})$. The lower bound (3.32) can also be deduced from the Rayleigh inequality by choosing zero components in the vector y such that $y^T A y = w^T A_{G_s} w$, where the vector w contains the non zero components of y and A_{G_s} is the subgraph obtained by deleting those rows and columns that correspond to the zero components in y.

We remark that the largest eigenvalue of a non negative matrix, that is not necessarily symmetric, also obeys the Rayleigh principle (8.28) as can be verified from **art.** 152 by incorporating the Perron Frobenius Theorem 38. Hence, most of the deduced bounds in this Section 3.4 also apply to directed graphs, whose adjacency matrix is generally non symmetric.

44. Applying the Rayleigh's inequalities to A^k and using **art.** 144 and (3.8) leads to

$$\lambda_1 \geq \left(\frac{u^T A^k u}{u^T u} \right)^{\frac{1}{k}} = \left(\frac{N_k}{N} \right)^{\frac{1}{k}} \tag{3.33}$$

For example, for $k = 2$, **art.** 33 shows that

$$\lambda_1 \geq \sqrt{\frac{1}{N} \sum_{k=1}^{N} d_k^2} = \sqrt{\text{Var}[D] + (E[D])^2} = \frac{2L}{N} \sqrt{1 + \frac{\text{Var}[D]}{(E[D])^2}} \tag{3.34}$$

because the variance $\text{Var}[D] \geq 0$ and $\text{Var}[D]$ is only zero for regular graphs. The lower bound (3.34) is thus always better than the classical bound (3.31) for non regular graphs.

From the inequality (3.14) in **art.** 33, we deduce that

$$\left(\frac{N_k}{N} \right)^{\frac{1}{k}} \leq \left(\frac{N_{2k}}{N} \right)^{\frac{1}{2k}}$$

Since the sequence $\frac{N_1}{N}, \left(\frac{N_2}{N} \right)^{\frac{1}{2}}, \left(\frac{N_4}{N} \right)^{\frac{1}{4}}, \ldots$ is generally non decreasing, while each term is bounded by λ_1, we arrive at

$$\lim_{k \to \infty} \left(\frac{N_k}{N} \right)^{\frac{1}{k}} = \lambda_1$$

45. *Variations on the Rayleigh inequality.* A series of other bounds can be deduced from the Rayleigh inequality $\lambda_1 \geq \frac{y^T A y}{y^T y}$.

By choosing the vector $y = \left(d_1^\beta, d_2^\beta, \ldots, d_N^\beta \right)$ for some real number β, we have

$$\lambda_1 \geq \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} d_i^\beta d_j^\beta}{\sum_{k=1}^{N} d_k^{2\beta}} = \frac{\sum_{i=1}^{N} \sum_{j \in \text{ neighbors}(i)} (d_i d_j)^\beta}{\sum_{k=1}^{N} d_k^{2\beta}}$$

Maximizing the lower bound for β is difficult. The basic law of the degree (2.3) suggests to take $\beta = \frac{1}{2}$,

$$\lambda_1 \geq \frac{1}{L} \sum_{\text{all pairs } (i,j) \text{ of neighbors}} \sqrt{d_i d_j}$$

From (1.3), we deduce $\lambda_1 (x_1)_j \leq d_j \max_{l \text{ is a direct neighbor of } j} (x_1)_l$ for any node j. Thus, for any two nodes j and k, it holds that

$$\lambda_1^2 \leq d_j d_k \frac{\max_{l \text{ is a direct neighbor of } j} (x_1)_l}{(x_1)_j} \frac{\max_{m \text{ is a direct neighbor of } k} (x_1)_m}{(x_1)_k}$$

When choosing the pair (j,k) such that $(x_1)_j = \max_{m \text{ is a direct neighbor of } k} (x_1)_m$ and $(x_1)_k = \max_{l \text{ is a direct neighbor of } j} (x_1)$, we find that

$$\lambda_1 \leq \max_{\text{all pairs } (i,j) \text{ of neighbors}} \sqrt{d_i d_j}$$

Combining both bounds as

$$\frac{1}{L} \sum_{\text{all pairs } (i,j) \text{ of neighbors}} \sqrt{d_i d_j} \leq \lambda_1 \leq \max_{\text{all pairs } (i,j) \text{ of neighbors}} \sqrt{d_i d_j}$$

yields the improvement of the analogous classical inequalities $E[D] \leq \lambda_1 \leq d_{\max}$.

Choosing $\beta = 1$, equivalent to $y = d$ in Rayleigh's inequality, yields (**art. 33**)

$$\lambda_1 \geq \frac{d^T A d}{d^T d} = \frac{N_3}{N_2}$$

This bound is the special case for $m = 1$ of

$$\lambda_1 \geq \frac{u^T A^{2m+1} u}{u^T A^{2m} u} = \frac{N_{2m+1}}{N_{2m}} \tag{3.35}$$

which is obtained from Rayleigh's inequality for $y = A^m u$. The classical bound (3.31) is recovered when $m = 0$.

Invoking (3.13) yields for any non negative integer j and k

$$\frac{N_{k+j}}{N_k} = \lambda_1^j \frac{1 + S(k+j)}{1 + S(k)} = \lambda_1^j \left(1 - \frac{S(k) - S(k+j)}{1 + S(k)}\right) \tag{3.36}$$

where

$$S(k) = \sum_{n=2}^{N} \left(\frac{\lambda_n}{\lambda_1}\right)^k \frac{\cos^2 \alpha_n}{\cos^2 \alpha_1} = \sum_{\lambda_n > 0} \left(\frac{\lambda_n}{\lambda_1}\right)^k \frac{\cos^2 \alpha_n}{\cos^2 \alpha_1} + \sum_{\lambda_n < 0} \left(\frac{\lambda_n}{\lambda_1}\right)^k \frac{\cos^2 \alpha_n}{\cos^2 \alpha_1} \tag{3.37}$$

Assuming that $\left|\frac{\lambda_n}{\lambda_1}\right| < 1$, which excludes bipartite graphs by Theorem 22, then (3.37) tends exponentially fast in k to zero. Hence, the sequence $\frac{N_j}{N}, \frac{N_{1+j}}{N_1}, \frac{N_{2+j}}{N_2}, \dots$ converges to λ_1^j. Excluding in the sequel regular graphs for which $S(k) = 0$ and bipartite graphs, we have that

$$S(k) - S(k+j) = \sum_{\lambda_n > 0} \left|\frac{\lambda_n}{\lambda_1}\right|^k \left|1 - \left|\frac{\lambda_n}{\lambda_1}\right|^j\right| \frac{\cos^2 \alpha_n}{\cos^2 \alpha_1}$$

$$+ (-1)^k \sum_{\lambda_n < 0} \left|\frac{\lambda_n}{\lambda_1}\right|^k \left(1 - (-1)^j \left|\left(\frac{\lambda_n}{\lambda_1}\right)^j\right|\right) \frac{\cos^2 \alpha_n}{\cos^2 \alpha_1}$$

which demonstrates for even $k = 2m \geq 0$ that $S(2m) - S(2m+j) > 0$. Since $1 + S(k) > 0$, we deduce from (3.36) that

$$\lambda_1^j \geq \frac{N_{2m+j}}{N_{2m}} \tag{3.38}$$

from which (3.35) follows alternatively. For odd $k = 2m + 1 \geq 1$ and odd j,

the sign of $S(k) - S(k+j)$ can be negative. Indeed, we can always rewrite (3.37) as an alternating series with non increasing (in absolute value) terms. If $\left|\frac{\lambda_{N\ 1}}{\lambda_1}\right|^k \frac{\cos^2 \alpha_{N\ 1}}{\cos^2 \alpha_1} > \left|\frac{\lambda_2}{\lambda_1}\right|^k \frac{\cos^2 \alpha_2}{\cos^2 \alpha_1}$, then

$$S(k) = -\left|\frac{\lambda_{N\ 1}}{\lambda_1}\right|^k \frac{\cos^2 \alpha_{N\ 1}}{\cos^2 \alpha_1} + \left|\frac{\lambda_2}{\lambda_1}\right|^k \frac{\cos^2 \alpha_2}{\cos^2 \alpha_1} - \left|\frac{\lambda_{N\ 2}}{\lambda_1}\right|^k \frac{\cos^2 \alpha_{N\ 2}}{\cos^2 \alpha_1} + \left|\frac{\lambda_3}{\lambda_1}\right|^k \frac{\cos^2 \alpha_3}{\cos^2 \alpha_1} + \ldots$$

and we have that

$$0 < \left|\frac{\lambda_{N\ 1}}{\lambda_1}\right|^k \frac{\cos^2 \alpha_{N\ 1}}{\cos^2 \alpha_1} - \left|\frac{\lambda_2}{\lambda_1}\right|^k \frac{\cos^2 \alpha_2}{\cos^2 \alpha_1} \le -S(k) \le \left|\frac{\lambda_{N\ 1}}{\lambda_1}\right|^k \frac{\cos^2 \alpha_{N\ 1}}{\cos^2 \alpha_1}$$

such that $S(k) < 0$ and, similarly, $S(k) - S(k+j) < 0$. In such a case and confining to $j = 1$, both the lower and upperbound,

$$\frac{N_{2m+1}}{N_{2m}} < \lambda_1 < \frac{N_{2m+2}}{N_{2m+1}}$$

converge with increasing m to λ_1.

By applying the inequality (Hardy *et al.*, 1999)

$$\min_{1 \le k \le n} \frac{a_k}{q_k} \le \frac{a_1 + a_2 + \cdots + a_n}{q_1 + q_2 + \cdots + q_n} \le \max_{1 \le k \le n} \frac{a_k}{q_k} \tag{3.39}$$

where $q_1, q_2, \ldots, q_n$ are positive real numbers and $a_1, a_2, \ldots, a_n$ are real numbers, we obtain

$$\frac{N_{2m+j}}{N_{2m}} = \frac{\sum_{n=1}^{N} \left(x_n^T u\right)^2 \lambda_n^{2m+j}}{\sum_{n=1}^{N} \left(x_n^T u\right)^2 \lambda_n^{2m}} \le \max_{1 \le n \le N} \frac{\left(x_n^T u\right)^2 \lambda_n^{2m+j}}{\left(x_n^T u\right)^2 \lambda_n^{2m}} = \lambda_1^j$$

establishing the inequality (3.38) again. For example, since $S(2k + 2j) < S(2k)$, for $j = 2$, the sequence $\frac{N_2}{N_0} \le \frac{N_4}{N_2} \le \frac{N_6}{N_4} \le \ldots$ monotonously increases towards λ_1^2.

46. *Optimized Rayleigh lower bounds.* Yet another choice is $y = u + \beta d$, where the parameter β will be tuned to maximize the Rayleigh lower bound. Introducing this vector y into Rayleigh's inequality $\lambda_1 \ge \frac{y^T A y}{y^T y}$ leads to

$$\lambda_1 \ge \frac{2L + 2\beta d^T d + \beta^2 d^T A d}{N + 4\beta L + \beta^2 d^T d} = \frac{N_1 + 2\beta N_2 + \beta^2 N_3}{N_0 + 2\beta N_1 + \beta^2 N_2}$$

where we have used $N = N_0$, $2L = u^T d = N_1$, $d^T d = N_2$ and $d^T A d = u^T A^3 u = N_3$, as shown in **art.** 33. The zeros of the denominator $N_0 + 2\beta N_1 + \beta^2 N_2 = 0$ are

$$\beta_{1,2} = \frac{-N_1 \pm \sqrt{N_1^2 - N_0 N_2}}{N_2}$$

The inequality (3.14) shows that $N_1^2 - N_0 N_2 \le 0$, implying that the zeros of the denominator are complex (unless for regular graphs). Maximizing the lower bound for β yields, after a tedious calculation,

$$\lambda_1 \ge \frac{N_0 N_3 - N_1 N_2 + \sqrt{N_0^2 N_3^2 - 6N_0 N_1 N_2 N_3 - 3N_1^2 N_2^2 + 4\left(N_1^3 N_3 + N_0 N_2^3\right)}}{2\left(N_0 N_2 - N_1^2\right)} \tag{3.40}$$

Numerical results in Table 3.1 and Fig. 7.6 show that this bound is better than (3.34), which is not surprising because it includes via N_3 additional information about the graph.

	Air transport	Random ER	Complete bipartite
λ_1 exact	80.9576	19.3405	105.5557
bound (3.31) $= \frac{2L}{N}$	18.3079	18.3304	17.8701
bound (3.34)	42.7942	18.8005	105.5557
bound (3.40)	75.9029	19.2867	105.5557

Table 3.1. *Comparison of a few lower bounds for λ_1. All networks have $N = 1247$ nodes. The European direct airport to airport traffic network is obtained from Eurostat, while the Erdős Rénji graph is defined in Section 1.3 and the complete bipartite graph $K_{n,m}$ in Section 5.7.*

From a computational point of view, given the $N \times N$ adjacency matrix A, the number of elementary computations for N_k is about $O\left(N^2\right)$, because it is the addition of the computational complexity of A^2, which is $O\left(N^2\right)$, and that of $A^3 = AA^2$, which is another $O\left(N^2\right)$, and so on, and that of $N_k = u^T A^k u$, which is again $O\left(N^2\right)$. On the other hand (see Golub and Van Loan (1996)), a full eigenvalue decomposition of A requires at most $O\left(N^3\right)$ elementary operations.

An extension of the last approach is to choose the vector

$$y = \sum_{j=0}^{m} A^j u \, \beta_j$$

such that Rayleigh's inequality becomes

$$\lambda_1 \geq \frac{\sum_{j=0}^{m} \sum_{k=0}^{m} \beta_j \beta_k u^T A^{j+k+1} u}{\sum_{j=0}^{m} \sum_{k=0}^{m} \beta_j \beta_k u^T A^{j+k} u} = \frac{\sum_{j=0}^{m} \sum_{k=0}^{m} \beta_j \beta_k N_{j+k+1}}{\sum_{j=0}^{m} \sum_{k=0}^{m} \beta_j \beta_k N_{j+k}}$$

The right hand side is a multi dimensional function that, in principle, can be opti mized for $\beta_1, \beta_2, \ldots, \beta_m$.

47. *Rayleigh's inequality and the walk generating function.* Continuing as in **art.** 45, we now propose to choose in the Rayleigh inequality $\lambda_1 \geq \frac{y^T A y}{y^T y}$, the vector

$$y = \sum_{j=0}^{\infty} A^j u \, z^j = u + zd + z^2 A d + \ldots$$

which converges for $|z| < \lambda_1^{-1}$ (**art.** 34). Using the Cauchy product of power series

yields

$$
y^T y = \sum_{m=0}^{\infty} u^T A^m \, z^m \sum_{j=0}^{\infty} A^j u \, z^j = \sum_{k=0}^{\infty} \left(\sum_{m=0}^{k} u^T A^{k\,-m} A^m u \right) z^k
$$

$$
= \sum_{k=0}^{\infty} (k+1) \, u^T A^k u \, z^k
$$

Written in terms of the generating function (3.15) of the total number of walks in a graph G results in

$$
y^T y = \sum_{k=0}^{\infty} (k+1) \, N_k z^k = \frac{d}{dz} \left(z N_G \left(z \right) \right)
$$

Similarly, we find that

$$
y^T A y = \sum_{k=0}^{\infty} (k+1) \, N_{k+1} z^k = \frac{dN_G \left(z \right)}{dz}
$$

Rayleigh's inequality becomes, for $|z| < \lambda_1{}^1$,

$$
\lambda_1 \geq \frac{\frac{dN_G(z)}{dz}}{\frac{d}{dz} \left(z N_G \left(z \right) \right)} = \frac{\frac{dN_G(z)}{dz}}{z \frac{dN_G(z)}{dz} + N_G \left(z \right)} \tag{3.41}
$$

For example, for regular graphs, whose generating function (3.19) of the total num ber walks is particularly simple, equality in (3.41) is established for all $|z| < \lambda_1{}^1$. Conversely, the solution of the differential equation deduced from (3.41) with equal ity sign is precisely the generating function (3.19) of regular graphs. When $z = 0$, (3.41) reduces to $\lambda_1 \geq \frac{N_1}{N}$, which is the classical lower bound (3.31).

For small z, we substitute the power series of $N_G \left(z \right)$ up to order three in z in the right hand side of (3.41),

$$
\lambda_1 \geq \frac{N_1 + 2N_2 z + 3N_3 z^2 + O \left(z^3 \right)}{N_0 + 2N_1 z + 3N_2 z^2 + O \left(z^3 \right)}
$$

which shows that the right hand side is similar to the β variant in **art.** 45 that led to (3.40) and that it increases from 0 with z, because $N_3 > N_2 > N_1 > N_0$. The function on the right hand side of (3.41) is thus maximal when

$$
N_G \left(z \right) \frac{d^2 N_G \left(z \right)}{dz^2} = 2 \left(\frac{dN_G \left(z \right)}{dz} \right)^2
$$

whose solution for real z, provided $N_G \left(z \right)$ is known, will lead to the best lower bound for λ_1 in (3.41). On the other hand, this differential equation can be solved for $N_G \left(z \right)$. Rewritten as

$$
\frac{1}{\frac{dN_G(z)}{dz}} \frac{d^2 N_G \left(z \right)}{dz^2} = \frac{2}{N_G \left(z \right)} \frac{dN_G \left(z \right)}{dz}
$$

and integrating both sides from 0 to z gives

$$\log \frac{dN_G(z)}{dz} - \log \frac{dN_G(z)}{dz}\bigg|_{z=0} = 2\left(\log \frac{N_G(z)}{N_G(0)}\right)$$

Using $N_G(0) = N$ and $\frac{dN_G(z)}{dz}\big|_{z=0} = N_1 = 2L$, we obtain after simplification,

$$\frac{dN_G(z)}{(N_G(z))^2} = \frac{2L}{N^2} dz$$

After integrating both sides for 0 to z and after some rearrangement, we arrive at

$$N_G(z) = \frac{N}{1 - \frac{2L}{N} z}$$

which is, again, the generating function (3.19) of a regular graph because $E[D] = \frac{2L}{N} = r$.

At last, we can rewrite the inequality in (3.41) as

$$\lambda_1 \geq \frac{1}{z + \frac{N_G(z)}{\frac{dN_G(z)}{dz}}}$$

or

$$\frac{1}{\lambda_1} \leq z + \frac{1}{\frac{d \log N_G(z)}{dz}}$$

48. An improvement of the classical bound (3.31) in terms of the total number (3.8) of walks N_k is derived in Van Mieghem (2007) (and improved in Walker and Van Mieghem (2008)),

$$\lambda_1 \geq \frac{N_1}{N} + 2\left(\frac{N_3}{2N} - \frac{N_1 N_2}{N^2} + \frac{N_1^3}{2N^3}\right)\lambda_0^{\,2} + O(t^{\,4}) \tag{3.42}$$

where $t \geq T$, $\lambda_0 = t\sqrt{N}$,

$$T = \frac{1}{\sqrt{N}} \max_{1 \leq j \leq m}\left(a_{jj} + \sum_{i \neq j}|a_{ij}|\right) \tag{3.43}$$

Since $N_1 = u^T A u = 2L$, the first term in (3.42) is the classical bound (3.31). The Lagrange series (3.42) with terms containing powers of $\lambda_0^{\,2j}$ for $j > 0$ measures the irregularity $\lambda_1 - E[D]$ of the graph.

49. A direct consequence of **art.** 24 is that the largest eigenvalue λ_1 is bounded by

$$\lambda_1 \leq \sqrt{\frac{2L(N-1)}{N}} \tag{3.44}$$

and equality in (3.44) occurs for the complete graph K_N (see Section 5.1).

Alternatively, in terms of the average degree $d_a = \frac{1}{N}\sum_{j=1}^{N} d_j = \frac{2L}{N}$, the largest eigenvalue λ_1 is bounded by the geometric mean of the average degree and the

maximum possible degree, $\lambda_1 \leq \sqrt{d_a (N-1)}$. Combining the lower bound (3.34) and upper bound (3.44) with **art. 23** yields

$$\frac{2L}{N} \sqrt{1 + \frac{\text{Var}[D]}{(E[D])^2}} \leq \lambda_1 \leq \min\left\{ \sqrt{\frac{2L(N-1)}{N}}, d_{\max} \right\} \tag{3.45}$$

More generally, combining Theorem 63, **art. 23** and **art. 44** gives for any integer $k \geq 1$

$$\left(\frac{N_{2k}}{N}\right)^{\frac{1}{2k}} \leq \lambda_1 \leq \min\left\{ \left(\frac{W_{2k}}{1 + (N-1)^{1-2k}}\right)^{\frac{1}{2k}}, d_{\max} \right\} \tag{3.46}$$

where W_k is the number of closed walks with k hops. For $k = 1$, (3.46) reduces to (3.45).

When we assume that $\left|\frac{\lambda_n}{\lambda_1}\right| < 1$ for all $2 \leq n \leq N$, which, as mentioned in **art. 45**, excludes bipartite graphs, the definition of W_k (**art. 36**) indicates that

$$W_k = \lambda_1^k \left\{ 1 + \sum_{j=2}^{N} \left(\frac{\lambda_j}{\lambda_1}\right)^k \right\} < \lambda_1^k \left\{ 1 + (N-1) \left|\frac{\max(\lambda_2, \lambda_N)}{\lambda_1}\right|^k \right\}$$

This implies that $W_k^{1/k}$ is decreasing in k, because $(1+x)^{1/k}$ is for $x > 0$ and, in addition, $\left(\frac{\max(\lambda_2, \lambda_N)}{\lambda_1}\right)^k$ is exponentially decaying in k. Hence, $\lim_{k\to\infty} W_k^{1/k} = \lambda_1$. While the left hand side of (3.46) is increasing in k (**art. 44**), the right hand side is decreasing in k. Together, they provide increasingly sharp bounds for λ_1 when k increases.

50. *Bounds for connected graphs.* As will be deduced in Section 4.1.1, a connected graph has an adjacency matrix that is irreducible (Section 8.5). We apply the bounds (8.54) in **art. 169** to A^2 by choosing $y = u$,

$$\min_{1 \leq i \leq N} \left(A^2 u\right)_i \leq \lambda_1^2 \leq \max_{1 \leq i \leq N} \left(A^2 u\right)_i$$

where $\left(A^2 u\right)_i = (Ad)_i = \sum_{j=1}^{N} a_{ij} d_j = \sum_{j \in \text{neighbors}(i)} d_j$. Thus,

$$\min_{1 \leq i \leq N} \sqrt{\sum_{j \in \text{neighbors}(i)} d_j} \leq \lambda_1 \leq \max_{1 \leq i \leq N} \sqrt{\sum_{j \in \text{neighbors}(i)} d_j} \tag{3.47}$$

Invoking the basic law of the degree (2.3), we have

$$\left(A^2 u\right)_i = 2L - d_i - \sum_{j \notin \text{neighbor}(i)} d_j \leq 2L - d_i - (N - 1 - d_i)$$

where the inequality arises from the connectivity of the graph, which implies that the degree d_j of each node j is at least one. Thus, $\max_{1 \leq i \leq N} \left(A^2 u\right)_i = 2L - N + 1$

and this maximum is reached in the complete graph K_N and in the star $K_{1,N\ 1}$. Hence, for any connected graph, we obtain the bound

$$\lambda_1 \leq \sqrt{2L - N + 1} \tag{3.48}$$

which is sharper than (3.44), but the latter bound did not assume connectivity of the graph.

When choosing $y = d$ in (8.54) in **art.** 169, we obtain a companion of (3.47) for connected graphs:

$$\min_{1 \leq i \leq N} \frac{1}{d_i} \sum_{j \in \text{neighbors}(i)} d_j \leq \lambda_1 \leq \max_{1 \leq i \leq N} \frac{1}{d_i} \sum_{j \in \text{neighbors}(i)} d_j \tag{3.49}$$

51. From the inequality (8.42) for Hölder q norms, we find for $p > q > 0$ that

$$\sum_{k=1}^{N} |\lambda_k|^q < \Lambda^q \quad \Rightarrow \quad \sum_{k=1}^{N} |\lambda_k|^p < \Lambda^p$$

Since $\sum_{k=1}^{N} \lambda_k = 0$, not all λ_k can be positive and combined with $\left|\sum_{k=1}^{N} \lambda_k^p\right| \leq \sum_{k=1}^{N} |\lambda_k|^p$, we also have that $\left|\sum_{k=1}^{N} \lambda_k^p\right| < \Lambda^p$. Applied to the case where $q = 2$ and $p = 3$ gives the following implication: if $\sum_{k=2}^{N} \lambda_k^2 < \lambda_1^2$ then $\left|\sum_{k=2}^{N} \lambda_k^3\right| < \lambda_1^3$. In that case, the number of triangles given in (3.3) is

$$\blacktriangle_G = \frac{1}{6}\lambda_1^3 + \frac{1}{6}\sum_{k=2}^{N} \lambda_k^3 \geq \frac{1}{6}\lambda_1^3 - \frac{1}{6}\left|\sum_{k=2}^{N} \lambda_k^3\right| > 0$$

Hence, if $2L = \sum_{k=2}^{N} \lambda_k^2 + \lambda_1^2 < 2\lambda_1^2$, then the number of triangles $\blacktriangle_G$ in G is at least one. Equivalently, in view of (3.2), if $\lambda_1 > \sqrt{L}$ then the graph G contains at least one triangle.

52. A theorem of Turan states that:

Theorem 9 *A graph G with N nodes and more than $\left[\frac{N^2}{4}\right]$ links contains at least one triangle.*

This theorem is a consequence of **art.** 51. For, using $L > \frac{N^2}{4} \geq \left[\frac{N^2}{4}\right]$, which is equivalent to $N < 2\sqrt{L}$ in the bound on the largest eigenvalue (3.31),

$$\lambda_1 \geq \frac{2L}{N} > \frac{2L}{2\sqrt{L}} = \sqrt{L}$$

and $\lambda_1 > \sqrt{L}$ is precisely the condition in **art.** 51 to have at least one triangle.

53. The graph formed by the union of all shortest hop paths, defined in **art.** 20, between node u and node v has at most $\left[\frac{N^2}{4}\right]$ links.

Indeed, the union of two shortest paths $\mathcal{P}_1$ and $\mathcal{P}_2$ between the same source destination pair cannot have a triangle. For, suppose that there were a triangle between three nodes i, j and k in the union $\mathcal{P}_1 \cup \mathcal{P}_2$. Since the link $i \rightarrow k$ is a

subsection of a shortest hop path, it obeys the strict triangle inequality (all $w = 1$ are the same),

$$w\,(i \rightarrow k) < w\,(i \rightarrow j) + w\,(j \rightarrow k)$$

otherwise the link $i \rightarrow k$ is not the shortest hop path from i to k. Hence, the sub section $i \rightarrow j \rightarrow k$ is not a shortest hop path. The triangle inequality thus implies that the union of the shortest hop paths between the same source destination pair cannot have a triangle. Turan's Theorem 9 then states that the number of links in that union is at most $\left[\frac{N^2}{4}\right]$.

54. We can deduce a set of lower bounds for λ_1 by considering (1.4). The Perron Frobenius theorem, as explained in **art.** 21, states that all eigenvector components are non negative, which leads in (1.4) to the bound

$$\lambda_1^m > (A^m)_{jj}$$

where $(A^m)_{jj}$ equals the number of closed m hop walks starting and ending at node j (see **art.** 17). Since the bound holds for any node j and any integer $m \geq 1$, we arrive at

$$\lambda_1 > \max_{m \geq 1} \sqrt[m]{\max_{1 \leq j \leq N} (A^m)_{jj}} \tag{3.50}$$

The largest eigenvalue of the adjacency matrix is at least as big as the m th root of the largest number of m hop cycles around a node in the graph. For example, invoking **art.** 30, (3.50) shows in the case $m = 2$ that $\lambda_1 > \sqrt{d_{\max}}$. The lower bound (3.50) is, in general, weak. The related upper bound

$$\lambda_1 \leq \max_{m \geq 1} \sqrt[m]{\max_{1 \leq i \leq N} \sum_{j=1}^{N} (A^m)_{ij}}$$

follows from (8.51) and (8.47). Since $W_m = \sum_{j=1}^{N} (A^m)_{jj}$, the above upper bound is different from (3.46).

3.5 Eigenvalue spacings

The difference $\lambda_k - \lambda_{k+1}$, for $1 \leq k \leq N-1$, between two consecutive eigenvalues of the adjacency matrix A is called the k th eigenvalue spacing of A. Only basic and simple, but general relations are deduced. Higher order differences (see **art.** 207) are not considered, nor the combination with the powerful Interlacing Theorem 42 in **art.** 180.

55. *Spectral gap.* The difference between the largest eigenvalue λ_1 and second largest λ_2, called the spectral gap, is never larger than N:

$$\lambda_1 - \lambda_2 \leq N \tag{3.51}$$

Indeed, since $\lambda_1 > 0$ as indicated by (3.45), it follows from (3.1) that

$$0 = \sum_{k=1}^{N} \lambda_k = \lambda_1 + \sum_{k=2}^{N} \lambda_k \leq \lambda_1 + (N-1)\lambda_2$$

such that

$$\lambda_2 \geq -\frac{\lambda_1}{N-1}$$

Hence,

$$\lambda_1 - \lambda_2 \leq \lambda_1 + \frac{\lambda_1}{N-1} = \frac{N\lambda_1}{N-1}$$

Art. 23 states that the largest possible eigenvalue is $\lambda_1 = N - 1$, attained in the complete graph, which proves (3.51). Again, the equality sign in (3.51) occurs in case of the complete graph (see Section 5.1). When a link is removed in the complete graph, the spectral gap drops by at least 1 (see Section 5.10). The spectral gap plays an important role in the dynamics of processes on graphs (**art.** 64) and it characterizes the robustness of a graph due to its relation with the algebraic connectivity (**art.** 74 and Section 4.2).

56. *Eigenvalue spacings.* The sum over all spacings between two consecutive eigenvalues equals

$$\sum_{k=1}^{N-1} (\lambda_k - \lambda_{k+1}) = \lambda_1 - \lambda_N \tag{3.52}$$

Since each spacing $\lambda_k - \lambda_{k+1} \geq 0$, the largest possible spacing occurs when all but one spacing is zero, in which case $\max_{1 \leq k \leq N-1} \lambda_k - \lambda_{k+1}$ is equal to $\lambda_1 - \lambda_N$. However, each spacing consists of two consecutive eigenvalues, which implies that $\lambda_N = \lambda_2$ (or $\lambda_{N-1} = \lambda_1$). **Art.** 55 shows that the largest possible spacing is attained in the complete graph and is equal to N, the largest possible spectral gap.

Let $\Delta\lambda$ denote an arbitrary spacing between two consecutive eigenvalues, then the telescoping series (3.52) shows that its average equals

$$E[\Delta\lambda] = \frac{\lambda_1 - \lambda_N}{N-1} \leq \frac{2d_{\max}}{N-1}$$

The variance $\text{Var}[\Delta\lambda] = E\left[(\Delta\lambda)^2\right] - (E[\Delta\lambda])^2$ is, however, more difficult to compute, because it requires the determination of the sum

$$E\left[(\Delta\lambda)^2\right] = \frac{1}{N-1} \sum_{k=1}^{N-1} (\lambda_k - \lambda_{k+1})^2$$

or equivalently, of the sum $\sum_{k=1}^{N-1} \lambda_k \lambda_{k+1}$.

Abel's partial summation

$$\sum_{k=1}^{n} a_k b_k = \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l\right)(b_k - b_{k+1}) + b_n \left(\sum_{l=1}^{n} a_l\right) \tag{3.53}$$

applied to (3.1) shows that

$$\sum_{k=1}^{N-1} k\left(\lambda_k - \lambda_{k+1}\right) = -N\lambda_N$$

Invoking (3.39) with $a_k = k\left(\lambda_k - \lambda_{k+1}\right)$ and $q_k = k$ yields bounds for the minimum and maximum spacing between consecutive eigenvalues of the adjacency matrix A:

$$0 \leq \min_{1 \leq k \leq N-1} \lambda_k - \lambda_{k+1} \leq \frac{-2\lambda_N}{N-1} \leq \max_{1 \leq k \leq N-1} \lambda_k - \lambda_{k+1} \tag{3.54}$$

Relation (8.57) in **art. 172** implies that

$$-\lambda_N \leq \left\lceil \frac{N}{2} \right\rceil$$

such that the minimum spacing is never larger than

$$\min_{1 \leq k \leq N-1} \lambda_k - \lambda_{k+1} \leq \frac{2}{N-1} \left\lceil \frac{N}{2} \right\rceil$$

57. *Inequalities for* λ_N. Besides the general bounds in **art. 172**, new bounds for the smallest eigenvalue λ_N of the adjacency matrix A can be deduced, when known relationships are rewritten in terms of the spacings.

Partial summation (3.53) of the total number of closed walks (3.24) yields, for any integer $0 \leq m \leq k$,

$$W_k = \sum_{j=1}^{N} \lambda_l^k = \sum_{j=1}^{N-1} \left(\sum_{l=1}^{j} \lambda_l^m \right) (\lambda_j^{k-m} - \lambda_{j+1}^{k-m}) + \lambda_N^{k-m} W_m \tag{3.55}$$

while the generalization of the telescoping series (3.52) is, for any n,

$$\sum_{j=1}^{N-1} \left(\lambda_j^n - \lambda_{j+1}^n \right) = \lambda_1^n - \lambda_N^n \tag{3.56}$$

The difference $\lambda_j^n - \lambda_{j+1}^n$ can be negative when eigenvalues are negative and n is even. The sum $\sum_{l=1}^{j} \lambda_l^m$ is always positive for $j < N$, which is immediate for even m. For odd m and denoting by q the index such that $\lambda_q \geq 0$ and $\lambda_{q+1} < 0$, we can write

$$\sum_{l=1}^{j} \lambda_l^m = \sum_{l=1}^{q} \lambda_l^m + \sum_{l=q+1}^{j} \lambda_l^m$$

where the first sum is strictly positive and the second is strictly negative. The sec ond sum decreases with increasing j, and is thus larger than or equal to $\sum_{l=q+1}^{N-1} \lambda_l^m$. However, in that extreme case where $j = N-1$, the sum $\sum_{l=1}^{N-1} \lambda_l^m = W_m - \lambda_N^m > 0$. The minimum value of the sum $\sum_{l=1}^{j} \lambda_l^m$ is attained for even m at $j = 1$ and for odd m at either $j = 1$, if $\lambda_1^m < W_m - \lambda_N^m$, or at $j = N-1$, if $\lambda_1^m > W_m - \lambda_N^m$. If

$m = 1$, the minimum occurs at $j = N - 1$ provided $\lambda_1 > |\lambda_N|$, which excludes, as in **art.** 45, bipartite graphs.

With this preparation, the inequality (3.39), with $a_j = q_j \sum_{l=1}^{j} \lambda_l^m$, $q_j = \lambda_j^{k}{}^{m} - \lambda_{j+1}^{k}{}^{m} > 0$ and $k - m$ is odd, becomes, using (3.55) and (3.56),

$$\frac{W_k - \lambda_N^{k}{}^{m} W_m}{\lambda_1^{k}{}^{m} - \lambda_N^{k}{}^{m}} \geq \min_{1 \leq j \leq N}{}_{1} \sum_{l=1}^{j} \lambda_l^m = \min\left(W_m - \lambda_N^m, \lambda_1^m\right) 1_{\{m \text{ is odd}\}} + \lambda_1^m 1_{\{m \text{ is even}\}}$$

from which we arrive at the bound, for even m and for odd m provided $W_m - \lambda_N^m > \lambda_1^m$,

$$\frac{W_k - \lambda_1^k}{W_m - \lambda_1^m} \geq \lambda_N^{k}{}^{m} \tag{3.57}$$

and, for odd m provided $W_m - \lambda_N^m < \lambda_1^m$,

$$\frac{W_k - \lambda_N^k}{W_m - \lambda_N^m} \geq \lambda_1^{k}{}^{m} \tag{3.58}$$

For example, for $k - m = 1$ and excluding bipartite graphs, (3.58) reduces for $k = 2$ and $m = 1$ and using (3.2) to

$$\frac{2L - \lambda_N^2}{-\lambda_N} \geq \lambda_1$$

from which we deduce that

$$\lambda_N \geq \frac{1}{2}\left(-\sqrt{\lambda_1^2 + 8L} + \lambda_1\right)$$

For $k = 3$ and $m = 2$, and using (3.3), (3.57) becomes

$$\frac{6\blacktriangle_G - \lambda_1^3}{2L - \lambda_1^2} \geq \lambda_N$$

Since we can only compute the sum $\sum_{j=1}^{N}{}^{1}\left(\sum_{l=1}^{j}\lambda_l^m\right)$ for $m = 0$, the inequality (3.39), with $a_j = q_j(\lambda_j^k - \lambda_{j+1}^k)$ and $q_j = j$, yields for all integer $k \geq 0$, using (3.55),

$$\min_{1 \leq j \leq N}{}_{1} \lambda_j^k - \lambda_{j+1}^k \leq \frac{2\left(W_k - N\lambda_N^k\right)}{N(N-1)} \leq \max_{1 \leq j \leq N}{}_{1} \lambda_j^k - \lambda_{j+1}^k \tag{3.59}$$

which is the generalization of (3.54). In particular, for odd values of $k = 2n + 1$, that conserve the ordering in the powers of eigenvalues, i.e., $\lambda_j^{2n+1} \geq \lambda_{j+1}^{2n+1}$ for all $1 \leq j \leq N - 1$, the bounds in (3.59) can be of interest.

3.6 Additional properties

58. *Cliques and cocliques.* A clique of size m in a graph G with $N \geq m$ nodes is a set of m pairwise adjacent nodes. Only when $m = N$ or the clique is a disjoint subgraph of G, the clique is a complete graph and each node has degree $m - 1$. A

coclique is the complement of a clique; thus, a set of pairwise non adjacent nodes. The clique number is the size of the largest clique, while the independence number is the size of the largest coclique.

Suppose that G has a coclique of size c. We can always relabel the nodes such that the nodes belonging to that coclique possess the first c labels. The corresponding adjacency matrix A has the form

$$A = \begin{bmatrix} O_{c \times c} & F_{c \times (N-c)} \\ F^T_{(N-c) \times c} & \tilde{F}_{(N-c) \times (N-c)} \end{bmatrix}$$

Since the principle matrix $O_{c \times c}$ has c eigenvalues equal to zero, the Interlacing Theorem 42 shows that, for $1 \leq j \leq c$,

$$\lambda_{N-c+j}(A) \leq 0 \leq \lambda_j(A)$$

Hence, the adjacency matrix has at least c non negative and $N - c + 1$ non positive eigenvalues. The converse is that the number $n_+ = \{j : \lambda_j(A) \geq 0\}$ of non negative eigenvalues of A provides an upper bound for the independence number. Also, the number $n_- = \{j : \lambda_j(A) \leq 0\}$ of non positive eigenvalues of A bounds the independence number by $N - n_-$.

Only for the complete graph K_N, where $c = 1$, there is only one positive eigen value. If one link (e.g. between node 1 and 2) in the complete graph is removed, the coclique has size $c = 2$, and two eigenvalues are non negative. Consequently, the second largest eigenvalue λ_2 in any graph apart from K_N is at least equal to zero. Another argument is that, apart from the complete graph, any graph possesses the star $K_{1,2}$ as a subgraph, whose adjacency eigenvalues are computed in Section 5.7. It follows then again from the Interlacing Theorem 42 that $\lambda_2 \geq 0$.

Similarly, if G has a clique of size c, then, after relabeling, the adjacency matrix has the form

$$A = \begin{bmatrix} (J-I)_{c \times c} & G_{c \times (N-c)} \\ G^T_{(N-c) \times c} & \tilde{G}_{(N-c) \times (N-c)} \end{bmatrix}$$

Since the principle matrix $(J - I)_{c \times c}$ has an eigenvalue $c - 1$ and $(-1)^{[c-1]}$ eigen values by (5.1), the Interlacing Theorem 42 shows that,

$$\lambda_{N-c+1}(A) \leq c - 1 \leq \lambda_1(A)$$

and, for $2 \leq j \leq c$,

$$\lambda_{N-c+j}(A) \leq -1 \leq \lambda_j(A)$$

The bounds for the clique are less elegant than those for the coclique.

59. Almost all non star like trees are *not* determined by the spectrum of the adja cency matrix (van Dam and Haemers, 2003). Godsil and Royle (2001) start by the remark that the spectrum of a graph does not determine the degrees, nor whether the graph is planar and that there are many graphs that are co spectral, i.e., al though graphs are different, their spectrum is the same. Cvetković *et al.* (2009)

devote a whole chapter on the characterization of graphs by their spectrum. They list theorems on graphs that are determined by their spectrum (such as regular graphs with degree $r = 2$ and complete bipartite graphs), but they also present counter examples. Finally, van Dam and Haemers (2003) conjecture that suffi ciently large graphs are determined by their spectrum, roughly speaking because the probability of having co spectral graphs becomes vanishingly small when the number of nodes N increases.

60. *Addition of a node to a graph.* When one node n is added to a graph G_N to form the graph G_{N+1}, the adjacency matrix of the latter is expressed as

$$A_{N+1} = \begin{bmatrix} A_N & v_{N\times 1} \\ (v^T)_{1\times N} & 0 \end{bmatrix} \tag{3.60}$$

where $v_{N\times 1}$ is the zero one connection vector of the new node n to any other node in G_N. The analysis below can be complemented with that in **art.** 181.

The characteristic polynomial of A_{N+1} is, invoking (8.79),

$$\det(A_{N+1} - \lambda I) = \det \begin{bmatrix} A_N - \lambda I & v \\ v^T & -\lambda \end{bmatrix}$$

$$= \det(A_N - \lambda I) \det\left(-\lambda - \left(v^T (A_N - \lambda I)^{-1} v\right)_{1\times 1}\right)$$

$$= -\left(\lambda + v^T (A_N - \lambda I)^{-1} v\right) \det(A_N - \lambda I)$$

With the expansion of the resolvent of A,

$$(A - \lambda I)^{-1} = -\frac{1}{\lambda}\left(I - \lambda^{-1} A\right)^{-1} = -\frac{1}{\lambda}\sum_{k=0}^{\infty} \frac{A^k}{\lambda^k} = -\frac{1}{\lambda}\left(I + \frac{A}{\lambda} + \frac{A^2}{\lambda^2} + \cdots\right) \tag{3.61}$$

we can write

$$v^T (A_N - \lambda I)^{-1} v = -\frac{1}{\lambda}\sum_{k=0}^{\infty} \frac{v^T A_N^k v}{\lambda^k} = -\frac{1}{\lambda}\left(d_n + \sum_{k=1}^{\infty} \frac{v^T A_N^k v}{\lambda^k}\right)$$

where $v^T v = d_n$ is the degree of node n. If we denote the characteristic polynomial of A_N by $c_{A_N}(\lambda) = \sum_{k=0}^{N} c_k(N) \lambda^k$, then we obtain

$$\sum_{k=0}^{N+1} c_k(N+1) \lambda^k = \left(-\lambda + \sum_{k=0}^{\infty} \frac{v^T A_N^k v}{\lambda^{k+1}}\right) \sum_{k=0}^{N} c_k(N) \lambda^k$$

$$= -\sum_{k=0}^{N} c_k(N) \lambda^{k+1} + \sum_{k=0}^{\infty}\sum_{j=0}^{N} c_j(N) \left(v^T A_N^k v\right) \lambda^{j\ k\ 1}$$

$$= -\sum_{k=1}^{N+1} c_{k\ 1}(N) \lambda^k + \sum_{m=\ \infty}^{N\ 1}\sum_{j=\max(0,m+1)}^{N} c_j(N) \left(v^T A_N^{j\ m\ 1} v\right) \lambda^m$$

Equating corresponding powers in λ yields[1], for $1 \leq k \leq N-1$, apart from $c_{N+1}(N+1) = (-1)^{N+1}$ and $c_N(N+1) = c_{N\ 1}(N) = 0$, a recursion that ex presses the coefficients of the characteristic polynomial of A_{N+1} in terms of those of A_N,

$$c_k(N+1) = -c_{k\ 1}(N) + \sum_{j=k+1}^{N} c_j(N)\left(v^T A_N^{j\ (k+1)} v\right)$$

while, for $k = 0$,

$$c_0(N+1) = \sum_{j=1}^{N} c_j(N)\left(v^T A_N^{j\ 1} v\right) = \det A_{N+1}$$

Given the coefficients $\{c_k(N)\}_{0 \leq k < N\ 1}$, the quadratic forms $r_k(v) = v^T A_N^k v$ for $1 \leq k < N$ constitute the major computational effort to determine the coeffi cients $\{c_k(N+1)\}_{0 \leq k < N}$. Starting with $N = 2$, the set can be iterated up to any size N and any structure in A_N, each N producing the set of coefficients $\{c_k(N)\}_{0 \leq k < N\ 1}$ of a polynomial with integer coefficients and real zeros lying in the interval $(-(N-1), N-1]$. Moreover, **art.** 180 shows that all eigenvalues of A_N interlace with those of A_{N+1}. These properties are also shared by orthogonal polynomials (see Chapter 10).

Suppose that v is an eigenvector of A with eigenvalue λ_v, then $\lambda_v = \lambda_{\max}(A_N) = \lambda_1$ by the Perron Frobenius Theorem 38 because v has non negative components[2]. Hence, if v is the eigenvector belonging to the largest eigenvalue and scaled to have only zero and one components, $A_N v = \lambda_1 v$ and $(A_N - \lambda I)^{\ 1} v = (\lambda_1 - \lambda)^{\ 1} v$ for $\lambda \neq \lambda_1$ such that

$$\left(v^T (A_N - \lambda I)^{\ 1} v\right)_{1 \times 1} = \frac{d_n}{\lambda_1 - \lambda}$$

and

$$\det(A_{N+1} - \lambda I) = \left(\lambda^2 - \lambda_1 \lambda - d_n\right) \frac{\det(A_N - \lambda I)}{\lambda_1 - \lambda}$$

Hence, if v is the (unscaled) eigenvector of A_N belonging to the largest eigenvalue whose norm is $\|v\|_2^2 = v^T v = d_n$, then the spectrum of A_{N+1} consists of all eigen values of A_N, except for $\lambda = \lambda_1$ and two new eigenvalues,

$$\frac{\lambda_1}{2}\left(1 \pm \sqrt{1 + 4\frac{d_n}{\lambda_1^2}}\right)$$

---

[1] Observe that, for $m < 0$, an identity is found because

$$v^T \left(\sum_{j\ 0}^{N} c_j(N) A_N^j\right) A_N^{-m-1} v \quad 0$$

by the Caley-Hamilton Theorem (**art.** 145), stating that $c_{A_N}(A_N) \quad \sum_{j\ 0}^{N} c_j(N) A_N^j \quad 0$.

[2] If v has zero components, then A is reducible, which implies that the graph G is disconnected.

In other words, the largest eigenvalue λ_1 of A_N is split up into a slightly larger one and a smaller one with strength related to the degree d_n. Such a vector v exists, for example, when $v = u$ and A_N is the adjacency matrix of a regular graph (**art.** 41).

61. Invoking (8.80), we obtain the alternative expression for the determinant

$$\det \begin{bmatrix} A_N - \lambda I & v_{N \times 1} \\ v^T & -\lambda \end{bmatrix} = -\lambda \det \left(A_N - \lambda I + \frac{vv^T}{\lambda} \right) \qquad (3.62)$$

For any complex number z, the determinant $\det(A_{N+1} - \lambda I)$ can be split into two others:

$$\det \begin{bmatrix} A_N - \lambda I & v_{N \times 1} \\ v^T & -\lambda \end{bmatrix} = \det \begin{bmatrix} A_N - \lambda I & v_{N \times 1} \\ v^T - w^T & -\lambda - z \end{bmatrix} + \det \begin{bmatrix} A_N - \lambda I & v_{N \times 1} \\ w^T & z \end{bmatrix}$$

The particular case where $v = w = u$, then reduces, for any $z \neq 0$, to

$$\det \begin{bmatrix} A_N - \lambda I & u_{N \times 1} \\ u^T & -\lambda \end{bmatrix} = \det \begin{bmatrix} A_N - \lambda I & u_{N \times 1} \\ u^T & z \end{bmatrix} - \det \begin{bmatrix} A_N - \lambda I & u_{N \times 1} \\ 0_{1 \times N} & \lambda + z \end{bmatrix}$$

When adding $-\frac{1}{z}$ times the last row to each other row in the first determinant, we obtain, with $J = u.u^T$,

$$\det(A_{N+1} - \lambda I) = z \det \left(A_N - \frac{1}{z} J - \lambda I \right) - (\lambda + z) \det(A_N - \lambda I) \qquad (3.63)$$

which reduces, for $z = -\lambda$, to (3.62). Since the adjacency matrix of the complement G^c equals $A^c = J - I - A$, choosing $z = 1$ in (3.63) results in

$$\det(A_{N+1} - \lambda I) = (-1)^N \det(A_N^c + (\lambda + 1) I) - (\lambda + 1) \det(A_N - \lambda I)$$

When a node that connects to all other nodes in G_N is added such that $v = u$, the resulting graph G_{N+1} is called the *cone* of G_N. The cone is always a connected graph. The cone construction is useful to convert a reducible matrix into an irreducible one, or to connect a graph with several disconnected clusters of components. An interesting application occurs in Google's PageRank as discussed in Van Mieghem (2006b, pp. 224 228). Finally, in case $v = u$, the quadratic forms in **art.** 60, $r_k(u) = u^T A_N^k u = N_k$, represent the total number of walks with k hops (**art.** 33).

62. If π is an equitable partition of the connected graph G, then the adjacency matrix A and the corresponding quotient matrix A^π have the same spectral radius.

Indeed, **art.** 15 shows that the eigenvalues of the quotient matrix corresponding to an equitable partition are a subset of the eigenvalues of the symmetric matrix. Moreover, any eigenvector v of A^π belonging to eigenvalue λ is transformed to an eigenvector Sv with the same eigenvalue λ. The Perron Frobenius Theorem 38 states that the eigenvector belonging to λ_1 is the only one with non negative components. Both A and A^π are non negative matrices. Since the characteristic matrix S of the partition has positive elements, both the eigenvector v and Sv have positive vector components and, thus, must belong to the spectral radius.

63. The spectral radius of any tree with maximum degree $d_{\max} > 1$ is smaller than $2\sqrt{d_{\max} - 1}$.

Indeed, Lemma 2 and 7 show that the spectral radius of any tree is at most equal to that of a centrally symmetric tree $T_{d_{\max}}$ as defined in **art. 16**. **Art. 62** allows us to concentrate on the quotient matrix A^π instead of the adjacency matrix. Gershgorin's Theorem 36, applied to the transformed quotient matrix $\widetilde{A^\pi}$ derived in **art. 16** shows that all eigenvalues are smaller than $2\sqrt{d_{\max} - 1}$ because $\frac{d_{\max}}{\sqrt{d_{\max} - 1}} < 2\sqrt{d_{\max} - 1}$ for $d_{\max} > 1$.

3.7 The stochastic matrix $P = \Delta^{-1}A$

64. The stochastic matrix $P = \Delta^{-1}A$, introduced in **art. 3**, characterizes a random walk on a graph. A random walk is described by a finite Markov chain that is time reversible. Alternatively, a time reversible Markov chain can be viewed as a random walk on an undirected graph. Random walks on graphs have many applications in different fields (see, e.g., the survey by Lovász (1993) and the relation with electric networks by Doyle and Snell (1984)); perhaps the most important application is randomly searching or sampling.

The combination of Markov theory and algebra leads to interesting properties of $P = \Delta^{-1}A$. The left eigenvector of P belonging to eigenvalue $\lambda = 1$ is the steady state vector π (which is a $1 \times N$ row vector, see Van Mieghem (2006b)). The corresponding right eigenvector is the all one vector u. These eigenvectors obey the eigenvalue equations $P^T \pi^T = \pi^T$ and $Pu = u$ and the orthogonality relation $\pi u = 1$ (**art. 140**). If $d = (d_1, d_2, \ldots, d_N)$ is the degree vector, then the basic law for the degree (2.5) is rewritten as $\left(\frac{d}{2L}\right)^T u = 1$. The steady state eigenvector π is unique (see Van Mieghem (2006b)) such that the equations $\pi u = 1$ and $\left(\frac{d}{2L}\right)^T u = 1$ imply that the steady state vector is

$$\pi = \left(\frac{d}{2L}\right)^T$$

or

$$\pi_j = \frac{d_j}{2L} \tag{3.64}$$

In general, the matrix P is not symmetric, but, after a similarity transform $H = \Delta^{1/2}$, a symmetric matrix $R = \Delta^{1/2} P \Delta^{-1/2} = \Delta^{-1/2} A \Delta^{-1/2}$ is obtained whose eigenvalues are the same as those of P (**art. 142**). The powerful property (**art. 151**) of symmetric matrices shows that all eigenvalues are real and that $R = U \operatorname{diag}(\lambda_R) U^T$, where the columns of the orthogonal matrix U consist of the normalized eigenvectors v_k that obey $v_j^T v_k = \delta_{jk}$. Explicitly written in terms of these eigenvectors gives (**art. 156**)

$$R = \sum_{k=1}^{N} \lambda_k v_k v_k^T$$

where, with the Perron Frobenius Theorem 38, the real eigenvalues are ordered as $1 = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \geq -1$. If we exclude bipartite graphs (where the set of nodes is $\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2$ with $\mathcal{N}_1 \cap \mathcal{N}_2 = \varnothing$ and where each link connects a node in $\mathcal{N}_1$ and in $\mathcal{N}_2$) or reducible Markov chains (**art. 167**), then $|\lambda_k| < 1$, for $k > 1$. **Art.** 142 shows that the similarity transform $H = \Delta^{1/2}$ maps the steady state vector π into $v_1 = H^{-1}\pi^T$ and, with (3.64),

$$v_1 = \frac{\Delta^{-1/2}\pi^T}{\left\|\Delta^{-1/2}\pi^T\right\|_2}$$

or

$$v_{1j} = \frac{\frac{\sqrt{d_j}}{2L}}{\sqrt{\sum_{j=1}^{N}\left(\frac{\sqrt{d_j}}{2L}\right)^2}} = \sqrt{\frac{d_j}{2L}} = \sqrt{\pi_j}$$

Finally, since $P = \Delta^{-1/2}R\Delta^{1/2}$, the spectral decomposition of the transition prob ability matrix of a random walk on a graph with adjacency matrix A is

$$P = \sum_{k=1}^{N}\lambda_k\Delta^{-1/2}v_kv_k^T\Delta^{1/2} = u\pi + \sum_{k=2}^{N}\lambda_k\Delta^{-1/2}v_kv_k^T\Delta^{1/2}$$

The n step transition probability is, with $\left(v_kv_k^T\right)_{ij} = v_{ki}v_{kj}$ and (3.64),

$$P_{ij}^n = \frac{d_j}{2L} + \sqrt{\frac{d_j}{d_i}}\sum_{k=2}^{N}\lambda_k^n v_{ki}v_{kj}$$

The convergence rate towards the steady state π_j, also coined the "mixing rate", can be estimated from

$$\left|P_{ij}^n - \pi_j\right| \leq \sqrt{\frac{d_j}{d_i}}\sum_{k=2}^{N}|\lambda_k^n|\,|v_{ki}|\,|v_{kj}| < \sqrt{\frac{d_j}{d_i}}\sum_{k=2}^{N}|\lambda_k^n|$$

Denoting by $\xi = \max\left(|\lambda_2|, |\lambda_N|\right)$ and by ξ_0 the largest element of the reduced set $\{|\lambda_k|\} \setminus \{\xi\}$ with $2 \leq k \leq N$, we obtain

$$\left|P_{ij}^n - \pi_j\right| < \sqrt{\frac{d_j}{d_i}}\xi^n + O\left(\xi_0^n\right)$$

Hence, the smaller ξ or, equivalently, the larger the spectral gap $|\lambda_1| - |\lambda_2| \geq 1 - \xi$, the faster the random walk converges to its steady state.

65. The stochastic matrix $P = \Delta^{-1}A$ can also be expressed in terms of the Lapla cian $Q = \Delta - A$ as $P = I - \Delta^{-1}Q$. This shows that the eigenvector x of P with corresponding eigenvalue λ is the same as that of the *normalized* Laplacian $\Delta^{-1}Q$ belonging to $\widetilde{\mu} = 1 - \lambda$ and $0 \leq \widetilde{\mu} \leq 2$. Hence, the spectral gap of a stochas tic matrix P also equals the second smallest eigenvalue of *normalized* Laplacian

$\Delta^{-1}Q$. Moreover, $\text{trace}(P) = \text{trace}(A) = 0$ and $\text{trace}(P^2) = \text{trace}(R^2)$ implies, with $(R)_{ij} = \frac{a_{ij}}{\sqrt{d_i d_j}}$, that

$$\sum_{k=1}^{N} \lambda_k^2(P) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{a_{ij}}{\sqrt{d_i d_j}} \frac{a_{ji}}{\sqrt{d_i d_j}} = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{a_{ij}}{d_i d_j}$$

With $\frac{1}{d_i d_j} = \frac{1}{2}\left\{ \frac{1}{d_i^2} + \frac{1}{d_j^2} - \left(\frac{1}{d_i} - \frac{1}{d_j}\right)^2 \right\}$, we obtain that

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \frac{a_{ij}}{d_i d_j} = \frac{1}{2}\sum_{i=1}^{N} \frac{1}{d_i^2} \sum_{j=1}^{N} a_{ij} + \frac{1}{2}\sum_{j=1}^{N} \frac{1}{d_j^2} \sum_{i=1}^{N} a_{ji} - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} a_{ij}\left(\frac{1}{d_i} - \frac{1}{d_j}\right)^2$$

$$= \sum_{i=1}^{N} \frac{1}{d_i} - \sum_{i=1}^{N}\sum_{j=1}^{i} a_{ij}\left(\frac{1}{d_i} - \frac{1}{d_j}\right)^2$$

Thus,

$$\sum_{k=1}^{N} \lambda_k^2(P) = \sum_{i=1}^{N} \frac{1}{d_i} - \sum_{i=1}^{N}\sum_{j=1}^{i} a_{ij}\left(\frac{1}{d_i} - \frac{1}{d_j}\right)^2$$

which shows that $\sum_{k=1}^{N} \lambda_k^2(P) \le \sum_{i=1}^{N} \frac{1}{d_i}$, where $\frac{1}{N}\sum_{i=1}^{N} \frac{1}{d_i}$ is the harmonic mean of the degree set $\{d_i\}_{1 \le i \le N}$. Only for regular graphs where $d_i = r$, the double sum disappears and $\sum_{k=1}^{N} \lambda_k^2(P) = \frac{N}{r}$. Since

$$\sum_{k=1}^{N} \lambda_k^2(P) = \sum_{k=1}^{N} \left(1 - \lambda_k\left(\Delta^{-1}Q\right)\right)^2 = 1 + \sum_{k=1}^{N-1} (1 - \widetilde{\mu}_k)^2$$

$$\le 1 + (N-1)(1 - \widetilde{\mu}_2)^2$$

we find, for regular graphs, an upper bound for the spectral gap $\widetilde{\mu}_2 \le 1 - \sqrt{\frac{N-r}{r(N-1)}}$. A tight upper bound

$$\widetilde{\mu}_2 \le 1 - 2\frac{\sqrt{d_{\max} - 1}}{d_{\max}}\left(1 - \frac{2}{\rho}\right) + \frac{2}{\rho}$$

for a graph with diameter $\rho \ge 4$ is derived by Nilli (1991) using Rayleigh's equation (4.12) and some ingenuity.

4

Eigenvalues of the Laplacian Q

In the sequel, we denote the eigenvalues of the Laplacian Q by μ to distinguish them from the eigenvalues λ of the adjacency matrix A.

4.1 General properties

66. The Laplacian $Q = \Delta - A$ is symmetric because A and Δ are both symmetric. Symmetry $Q = Q^T$ also follows from the other definition $Q = BB^T$.

The quadratic form defined in **art.** 160,

$$x^T Q x = x^T B B^T x = \left\| B^T x \right\|_2^2 \geq 0 \tag{4.1}$$

is positive semidefinite, which implies that all eigenvalues of Q are non negative and at least one is zero because $\det Q = 0$ as shown in **art.** 2. Thus, the zero eigenvalue is the smallest eigenvalue of Q. The eigenvector belonging to the zero eigenvalue is u because $\sum_{k=1}^{N} q_{ik} = 0$ for each row $1 \leq i \leq N$; in vector notation, $Qu = 0$.

We order the real, non negative eigenvalues of the Laplacian Q as $0 = \mu_N \leq \mu_{N\;1} \leq \cdots \leq \mu_1$. Similarly as for the adjacency matrix (**art.** 22), none of the eigenvalues of the Laplacian is a fraction of the form $\frac{a}{b}$, where a and b are co prime and $b > 1$. Only integer and irrational eigenvalues are possible.

67. Since Q is a symmetric matrix, all eigenvectors $x_1, x_2, \ldots, x_N$ are orthogonal (**art.** 151). **Art.** 66 shows that the eigenvector $x_N = u$ belonging to the smallest eigenvalue $\mu_N = 0$, such that, for all $1 \leq j \leq N - 1$,

$$u^T x_j = \sum_{k=1}^{N} (x_j)_k = 0$$

Thus, the sum of all vector components of an eigenvector, different from $x_N = u$, is zero. When these eigenvector components are ranked in increasing order, then the smallest and largest eigenvector component of $x_j \neq u$, with $1 \leq j \leq N - 1$, have a different sign.

68. Gerschgorin's Theorem 36 states that each eigenvalue μ of the Laplacian lies

in an interval $|\mu - d_j| \leq d_j$ around a degree d_j value. Hence,

$$0 \leq \mu \leq 2d_j$$

which shows that Gerschgorin's Theorem 36, alternatively to **art.** 66, demonstrates that Q is positive semidefinite. Moreover, $\mu_1 \leq 2d_{\max}$. This same bound (4.10) is also found by considering the non negative matrix $d_{\max}I - Q$ whose largest eigen value is $d_{\max}$ and smallest eigenvalue is $d_{\max} - \mu_1$. The Perron Frobenius Theorem 38 states that the positive largest eigenvalue is larger than the absolute value of any other one eigenvalue, whence $d_{\max} \geq |d_{\max} - \mu_1|$. This inequality is essentially the same as Gerschgorin's and, thus, it implies (4.10).

69. The definition of $Q = \Delta - A$ and (3.1) show that $\text{trace}(Q) = \text{trace}(\Delta) = \sum_{j=1}^{N} d_j$. The basic law of the degree (2.3) and relation (8.7) combine to

$$\sum_{k=1}^{N} \mu_k = 2L \qquad (4.2)$$

Hence, the average value of a Laplacian eigenvalue equals the average degree, $E[\mu] = E[D]$.

Corollary 1 shows that any partial sum with $1 \leq j \leq N$ of ordered eigenvalues satisfies

$$\sum_{k=1}^{j} d_{(k)} \leq \sum_{k=1}^{j} \mu_k \qquad (4.3)$$

where $d_{(k)}$ denotes the k th largest degree in the graph, i.e., $d_{(N)} \leq d_{(N\ 1)} \leq \cdots \leq d_{(1)}$.

70. Applying the general relation (8.20) to the Laplacian yields

$$\sum_{k=1}^{N} \mu_k^2 = \text{trace}\left(Q^2\right)$$

The square equals

$$Q^2 = (\Delta - A)^2 = \Delta^2 + A^2 - \left(\Delta A + (\Delta A)^T\right)$$

such that

$$\text{trace}\left(Q^2\right) = \sum_{k=1}^{N} d_k^2 + \text{trace}\left(A^2\right)$$

Using (3.5) leads to

$$\sum_{k=1}^{N} \mu_k^2 = \sum_{k=1}^{N} d_k^2 + 2L \qquad (4.4)$$

Stochastically[1], when considering the eigenvalue μ and the degree D in a graph as a random variable, (4.4) translates to

$$\mathrm{Var}\,[\mu] = \mathrm{Var}\,[D] + E\,[D]$$

where the variance $\mathrm{Var}[X] = E\,[X^2] - (E\,[X])^2$ for any random variable X. Since $E\,[D] > 0$ (excluding graphs without links), the variability of the Laplacian eigen values is larger than that of the degree D in the graph.

Applying Corollary 1 yields, for $1 \le j \le N$,

$$\sum_{k=1}^{j} d_{(k)}^2 + \sum_{k=1}^{j} d_{(k)} \le \sum_{k=1}^{j} \mu_k^2 \tag{4.5}$$

where $d_{(k)}$ denotes the k th largest degree in the graph.

71. The case for the third powers in (8.20) needs the computation of the trace of

$$Q^3 = (\Delta - A)^3$$
$$= \Delta^3 - \Delta^2 A - \Delta A \Delta + \Delta A^2 - A\Delta^2 + A\Delta A + A^2\Delta - A^3$$

Since $a_{jj} = 0$, all matrices to first power in A have a vanishing trace. By computing the product of the matrices, we find that

$$\mathrm{trace}\left(\Delta A^2\right) = \mathrm{trace}\left(A\Delta A\right) = \mathrm{trace}\left(A^2\Delta\right) = \sum_{k=1}^{N} d_k^2$$

Hence,

$$\mathrm{trace}\left(Q^3\right) = \sum_{k=1}^{N} d_k^3 + 3\sum_{k=1}^{N} d_k^2 - \mathrm{trace}\left(A^3\right)$$

where

$$\mathrm{trace}\left(A^3\right) = \sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N} a_{jk}a_{kl}a_{lj} = \sum_{k=1}^{N} \lambda_k^3$$

and (3.3) shows that $\mathrm{trace}(A^3)$ equals six times the number of triangles in the graph, which we denote by $\blacktriangle_G$. Combining all yields

$$\sum_{k=1}^{N} \mu_k^3 = \sum_{k=1}^{N} d_k^3 + 3\sum_{k=1}^{N} d_k^2 - 6\blacktriangle_G \tag{4.6}$$

For the complete graph, we have that $\mathrm{trace}(A^3) = N(N-1)(N-2)$ and $\sum_{k=1}^{N} d_k^2 = N(N-1)^2$ such that, for $N > 3$,

$$3\sum_{k=1}^{N} d_k^2 - 6\blacktriangle_G = 3N(N-1)(3-N) < 0$$

---

[1] Each of the values $\mu_1, \mu_2, \ldots, \mu_N$ is interpreted as a realization (outcome) of the random variable μ and the mean of the m-th powers is computed as $E\,[\mu^m] \quad \frac{1}{N}\sum_{k=1}^{N} \mu_k^m$.

while for a tree, where $\blacktriangle_G = 0$, the last two sums are $3\sum_{k=1}^{N} d_k^2 - 6\blacktriangle_G > 0$. Thus, the sum of the third powers of the Laplacian eigenvalues can be lower and higher than the corresponding sum of the degrees.

Stochastically, the third centered moment, which quantifies the skewness of the distribution, follows from (4.6) and (4.4) as

$$E\left[(\mu - E\,[\mu])^3\right] = E\left[(D - E\,[D])^3\right] + 3\mathrm{Var}\,[D] - \frac{6\blacktriangle_G}{N}$$

The third centered moment of the Laplacian eigenvalue μ differs from that of the degree D by an amount $3\left(\mathrm{Var}\,[D] - \frac{2\blacktriangle_G}{N}\right)$.

72. We can extend the previous computation to higher powers and compute, for any integer $m \geq 0$,

$$\mathrm{trace}\,(Q^m) = \mathrm{trace}\,((\Delta - A)^m)$$

by using the linearity and commutativity of the trace of the matrix product

$$\mathrm{trace}\,(CD) = \mathrm{trace}\,(DC)$$

When expanding the product $(\Delta - A)^m$ in a sum of 2^m matrix products[2] and applying the commutativity of the trace, we find the usual binomial expansion

$$\mathrm{trace}\,((\Delta - A)^m) = \sum_{k=0}^{m} \binom{m}{k}(-1)^{m-k}\,\mathrm{trace}\,(\Delta^k A^{m-k})$$

Since $\Delta^k = \mathrm{diag}\left(d_1^k, d_2^k, \ldots, d_N^k\right)$, we have that

$$\mathrm{trace}\,(\Delta^k A^{m-k}) = \sum_{l=1}^{N}\left(\Delta^k A^{m-k}\right)_{ll} = \sum_{l=1}^{N}\sum_{q=1}^{N}\left(\Delta^k\right)_{lq}\left(A^{m-k}\right)_{ql}$$

$$= \sum_{l=1}^{N} d_l^k \left(A^{m-k}\right)_{ll}$$

and

$$\mathrm{trace}\,(Q^m) = \sum_{k=0}^{m} \binom{m}{k}(-1)^{m-k} \sum_{l=1}^{N} d_l^k \left(A^{m-k}\right)_{ll}$$

Taking into account that $A_{ll} = 0$, we can express, using (8.20), the m th moment of the Laplacian eigenvalues in terms of the degree sequence and the number of closed walks $\left(A^j\right)_{ll}$ of length j starting and returning at node l (**art. 17**), as

$$\sum_{k=1}^{N} \mu_k^m = \sum_{l=1}^{N} d_l^m + \binom{m}{2}\sum_{l=1}^{N} d_l^{m-1} + \sum_{k=1}^{m-2}\binom{m}{k}(-1)^{m-k}\sum_{l=1}^{N} d_l^k \left(A^{m-k}\right)_{ll} + (-1)^m W_m$$

$$(4.7)$$

where we have introduced $W_k = \mathrm{trace}\left(A^k\right)$ as defined in **art. 36**.

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[2] Each product can be associated with a binary expression of a number $0 \leq j \leq 2^m$, in which a zero bit is replaced by the matrix Δ and a one bit by the matrix A.

73. Art. 158 relates the diagonal elements of a symmetric matrix to its eigen values and so provides another relation between the degree d_j of node j and the set of Laplacian eigenvalues $0 = \mu_N \leq \mu_{N-1} \leq \cdots \leq \mu_1$. The matrix equation (8.35) becomes $Y\mu = d$, where the vector $\mu = (\mu_1, \mu_2, \ldots, \mu_N)$, $d = (d_1, d_2, \ldots, d_N)$ and where the non negative matrix $Y^T = \begin{bmatrix} y_1 & y_2 & \cdots & y_N \end{bmatrix}$ consists of col umn vectors $y_j = (x_{1j}^2, x_{2j}^2, \ldots, x_{Nj}^2)$, where x_{kj} is the j th component of the k th eigenvector of Q belonging to μ_k.

Analogously to the adjacency matrix in **art. 32**, also for the Laplacian the deter minant is singular, $\det Y = 0$. This follows from (8.37) and the fact that $y_N = \frac{1}{N}u$, because the sum of the first $N-1$ columns in Y^T is a multiple of the last column. Hence, beside the largest eigenvalue at 1, Y (and Y^T) has also a zero eigenvalue. The obvious consequence is that $Y\mu = d$ cannot be inverted to $d = Y^{-1}\mu$. However, when deleting the last column and last row, the resulting matrix $\tilde{Y}$ (minor of Y) can be inverted and the degrees $d_1, d_2, \ldots, d_{N-1}$ can be determined. The degree d_N of the N th node then follows from the basic law (2.3).

74. If G is regular, where all nodes have the same degree, $d_j = r$ for all $1 \leq j \leq N$, then the eigenvalues of the Laplacian Q and the adjacency matrix A are directly connected because $\det(Q - \mu I) = \det((r - \mu)I - A)$. Thus, for all $1 \leq j \leq N$,

$$\mu_j(Q) = r - \lambda_{N+1-j}(A) \tag{4.8}$$

Since $\mu_N(Q) = 0$, we again find as in **art. 41** that the largest eigenvalue of the adjacency matrix in a regular graph equals $\lambda_1(A) = r$.

From (4.8), the difference for all $1 \leq j \leq N$,

$$\mu_{j-1}(Q) - \mu_j(Q) = \lambda_{N+1-j}(A) - \lambda_{N+2-j}(A)$$

shows that the spectral gap (**art. 55**) in a regular graph equals $\lambda_1(A) - \lambda_2(A) = \mu_{N-1}(Q)$. This relation might suggest that the spectral gap in any graph is related to the second smallest eigenvalue μ_{N-1} of the Laplacian, whose properties are further explored in Section 4.2. However, Section 7.5.2 exhibits a graph with large spectral gap and small μ_{N-1}.

75. A direct application of Lemma 8 to $A = \Delta - Q$ yields, for any eigenvalue $1 \leq k \leq N$,

$$d_{\min} - \mu_k(Q) \leq \lambda_k(A) \leq d_{\max} - \mu_k(Q)$$

and

$$d_{(k)} - \lambda_1(A) \leq \mu_k(Q) \leq d_{(k)} - \lambda_N(A)$$

Equality is only reached when $d_{\min} = d_{\max} = r$ as in a regular graph (**art. 74**).

76. *The Laplacian spectrum of the complement G^c of G.* From the adjacency matrix $A^c = J - I - A$ of the complement G^c of a graph G (**art. 1**), the Laplacian

of the complement G^c is immediate as

$$Q^c = \Delta^c - A^c = (N-1)I - \Delta - J + I + A$$
$$= NI - J - Q$$

Let $x_1, x_2, \ldots, x_N = u$ denote the eigenvectors of Q belonging to the eigenvalues $\mu_1, \mu_2, \ldots$, and $\mu_N = 0$, respectively. The eigenvalues of J are N and $[0]^{N-1}$ as shown in (5.1). Since $Ju = Nu$ and $Jx_j = 0$ for $1 \leq j \leq N-1$ as demonstrated in **art.** 85, we observe that

$$Q^c u = 0$$

and

$$Q^c x_j = (N - \mu_j) x_j$$

Hence, the set of eigenvectors of Q and of the complement Q^c are the same, while the ordered eigenvalues, for $1 \leq j \leq N-1$, are

$$\mu_j(Q^c) = N - \mu_{N-j}(Q) \tag{4.9}$$

Art. 66, and alternatively also **art.** 68, indicate that all eigenvalues of a Laplacian matrix are non negative, hence $\mu_j(Q^c) \geq 0$ for all $1 \leq j \leq N$ such that (4.9) then implies that $N - \mu_{N-j}(Q) \geq 0$, or that all Laplacian eigenvalues must lie in the interval $[0, N]$. Hence, the upper bound for μ_1 in **art.** 68 needs to be refined to

$$\mu_1 \leq \min(N, 2d_{\max}) \tag{4.10}$$

77. The Rayleigh's inequalities in **art.** 152 motivate us to consider the quadratic form (4.1) further. The l th component of $\left(B^T x\right)_l = x_i - x_j$ where the link $l = i \to j$ connects node i and j, starting at node $i = l^+$ and ending at node $j = l^-$. This observation allows us to write

$$x^T Q x = \left\| B^T x \right\|_2^2 = \sum_{l \in \mathcal{L}} (x_{l^+} - x_{l^-})^2 \tag{4.11}$$

Since the vector x consists of any real number, we may consider x as a real function $f(n)$ acting on a node n. Thus, with $x_{l^+} = f(l^+)$ and $x_{l^-} = f(l^-)$, we finally arrive at

$$(Qf, f) = \sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-) \right)^2$$

where $(g, f) = \sum_{x \in \mathcal{N}} f(x) g(x)$ denotes the scalar product (**art.** 241) of two real functions f and g belonging to $L^2(\mathcal{N})$, the space of all real functions on the set of nodes $\mathcal{N}$ for which the norm $\|f\|^2 = (f, f)$ exists.

78. Art. 67 shows that the eigenvector x of Q belonging to μ_{N-1} must satisfy $x^T u = 0$. By requiring this additional constraint and choosing the scaling of the

eigenvector such that $x^T x = 1$, Rayleigh's principle (**art.** 152) applied to the second smallest eigenvalue of the Laplacian results in

$$\mu_{N\ 1} = \min_{\|x\|_2^2 = 1 \text{ and } x^T u = 0} x^T Q x \tag{4.12}$$

Applied to the complement Q^c and with (4.9), we obtain

$$\mu_{N\ 1}(Q^c) = N - \mu_1(Q) = \min_{\|x\|_2^2 = 1 \text{ and } x^T u = 0} x^T Q^c x$$

Since $x^T Q^c x = x^T (NI - J - Q) x = N - x^T Q x$ as follows from **art.** 76, we obtain that

$$N - \mu_1(Q) = \min_{\|x\|_2^2 = 1 \text{ and } x^T u = 0} (N - x^T Q x) = N - \max_{\|x\|_2^2 = 1 \text{ and } x^T u = 0} x^T Q x$$

Hence, the largest eigenvalue of Q obeys

$$\mu_1(Q) = \max_{\|x\|_2^2 = 1 \text{ and } x^T u = 0} x^T Q x = N - \mu_{N\ 1}(Q^c)$$

4.1.1 Eigenvalues and connectivity

79. Disconnectivity is a special case of the reducibility of a matrix (**art.** 167) and expresses that no communication is possible between two nodes in a different component or cluster. A component of a graph G is a connected subgraph of G.

Theorem 10 *The graph G is connected if and only if $\mu_{N\ 1} > 0$.*

Proof: The theorem is a consequence of the Perron Frobenius Theorem 38 for a non negative, irreducible matrix. Indeed, consider the non negative matrix $\alpha I - Q$, where $\alpha \geq d_{\max}$. If G is connected, then $\alpha I - Q$ is irreducible and the Perron Frobenius Theorem 38 states that the largest eigenvalue r of $\alpha I - Q$ is positive and simple and the corresponding eigenvector x_r has positive components. Hence, $Q x_r = (\alpha - r) x_r$. Since eigenvectors of a symmetric matrix are orthogonal (**art.** 151) while $u^T x_r > 0$, x_r must be proportional to u, and thus $\mu_N = \alpha - r = 0$. Since there is only one such eigenvector x_r and since the eigenvalue r exceeds all others, all other eigenvalues of Q must exceed zero. $\square$

80. A graph G has k components (or clusters) if there exists a relabeling of the nodes such that the adjacency matrix has the structure

$$A = \begin{bmatrix} A_1 & O & \dots & O \\ O & A_2 & & \vdots \\ \vdots & & \ddots & \\ O & & \dots & A_k \end{bmatrix}$$

where the square submatrix A_m is the adjacency matrix of the connected component m. The corresponding Laplacian is

$$Q = \begin{bmatrix} Q_1 & O & \ldots & O \\ O & Q_2 & & \vdots \\ \vdots & & \ddots & \\ O & & \ldots & Q_k \end{bmatrix}$$

Using (8.79) indicates that

$$\det(Q - \mu I) = \prod_{m=1}^{k} \det(Q_m - \mu_m I)$$

Since each block matrix Q_m is a Laplacian, whose row sum is zero and $\det Q_m = 0$, the characteristic polynomial $\det(Q - \mu I)$ has at least a k fold zero eigenvalue. If each block matrix Q_m is irreducible, i.e., the m th cluster is connected, Theorem 10 shows that Q_m has only one zero eigenvalue. Hence, we have proved:

Theorem 11 *The multiplicity of the smallest eigenvalue $\mu = 0$ of the Laplacian Q is equal to the number of components in the graph G.*

If Q has only one zero eigenvalue with corresponding eigenvector u (**art. 66**), then the graph is connected; it has only one component. Theorem 11 as well as Theorem 10 also imply that, if the second smallest eigenvalue $\mu_{N\ 1}$ of Q is zero, the graph G is disconnected.

4.1.2 The number of spanning trees and the Laplacian Q

81. *Matrix Tree Theorem.* The coefficients $\{c_k(Q)\}_{0 \le k \le N}$ of the characteristic polynomial of the Laplacian

$$c_Q(x) = \det(Q - xI) = \sum_{k=0}^{N} c_k(Q) x^k$$

can be expressed in terms of sums over minors (see **art. 138**). Apart from $c_N = (-1)^N$, we apply (8.4) for $0 \le m < N$ to the Laplacian $Q = BB^T$

$$(-1)^{N\ m} c_{N\ m}(Q) = \sum_{all} \mathrm{minor}_m(BB^T) = \sum_{all} \det\left((BB^T)_m\right)$$

where $(Q)_m = (BB^T)_m$ denotes an $m \times m$ submatrix of Q obtained by deleting the same set of $N - m$ rows and columns and where the sum is of over all $\binom{N}{m} = \binom{N}{N\ m}$ ways in which $N - m$ rows can be deleted among the N rows. Since $Q = BB^T$ and $q_{ij} = \sum_{k=1}^{L} b_{ik} b_{jk}$, deleting a row i in Q translates to deleting row i in B. Thus, $(B)_m$ is an $m \times L$ submatrix of B in which the same $N - m$ rows in B are deleted.

We apply the Binet Cauchy Theorem 45 to $\det\left(BB^T\right)_m$. Using (8.85) gives

$$\det\left(BB^T\right)_m = \sum_{k_1=1}^{L} \sum_{k_2=k_1+1}^{L} \cdots \sum_{k_m=k_{m-1}+1}^{L} \begin{vmatrix} b_{1k_1} & \cdots & b_{1k_m} \\ \vdots & \cdots & \vdots \\ b_{mk_1} & \cdots & b_{mk_m} \end{vmatrix}^2$$

which illustrates that $\det\left(BB^T\right)_m$ is non zero so that $c_Q\left(-x\right)$ is a polynomial with positive coefficients. Descartes' rule (**art.** 212) shows that $c_Q\left(-x\right)$ has no real positive zero, agreeing with the non negativity of the Laplacian eigenvalues (**art.** 66). Poincaré's Theorem 2 tells us that the square of the above determinant in the multiple sum is either zero or one. It remains to investigate for which set $(k_1, k_2, \ldots, k_m)$ the determinant is non zero, hence, of rank m. **Art.** 6 shows that, only if the subgraph formed by the m links (columns in the matrix of the above determinant) is a spanning tree, the determinant is non zero.

To conclude, $\det\left(BB^T\right)_m$ equals the total number of trees with m links that can be formed in the graph on $m + 1$ given nodes. The coefficient $(-1)^{N-m} c_{N-m}\left(Q\right)$ then counts all these spanning trees with m links over all possible ways of deleting $N - m$ nodes in the graph. In summary, we have demonstrated the famous Matrix Tree Theorem:

Theorem 12 (Matrix Tree Theorem) *In a graph G with N nodes, the coefficient $(-1)^{N-m} c_{N-m}\left(Q\right)$ of the characteristic polynomial of the Laplacian Q equals the number of all spanning trees with m links in all subgraphs of G that are obtained after deleting $N - m$ nodes in all possible ways.*

Clearly, $c_0\left(Q\right) = \det Q = 0$ because there does not exist a tree with N links that spans the N nodes in a graph. The other extreme is, by convention, $(-1)^N c_N\left(Q\right) = 1$. Further, $(-1)^{N-1} c_{N-1}\left(Q\right) = 2L$, equals the number of spanning trees in G each consisting of one link, which equals twice the number of links in G. In deed, $\det\left(BB^T\right)_1 = \sum_{k_1=1}^{L} |b_{1k_1}|$ is the number of neighbors of node 1; taking the sum over all possible ways to delete one row results in $(-1)^{N-1} c_{N-1}\left(Q\right) = \sum_{i=1}^{N} \sum_{k_i=1}^{L} |b_{ik_i}|$, which is the sum of the absolute value of all elements in B. This result also follows from the general relation (8.7) for the second highest degree coefficient in any polynomial and **art.** 69. When $m = N - 1$, **art.** 6 shows that $\det\left(BB^T\right)_{N-1}$ equals the number of all spanning trees with $N - 1$ links in the graph G. Since there are precisely N ways to remove one node (one row in B), the coefficient $-c_1$ counts N times all trees spanning all N nodes in G.

The characteristic polynomial of the Laplacian of the example graph in Fig. 2.1 is

$$c_Q\left(x\right) = x^6 - 18x^5 + 125x^4 - 416x^3 + 659x^2 - 396x$$

$$= x\left(x - \frac{7 - \sqrt{13}}{2}\right)\left(x - \frac{7 - \sqrt{5}}{2}\right)(x - 4)\left(x - \frac{7 + \sqrt{5}}{2}\right)\left(x - \frac{7 + \sqrt{14}}{2}\right)$$

The example graph has 18 spanning trees with one link, 125 consisting of two links, ..., and 66 spanning trees with five links ($396 = 6 \times 66$).

There is another Matrix Tree Theorem variant for the coefficients of the characteristic polynomial of Q due to Kelmans and Chelnokov (1974) based on the notion of a forest. A forest is a collection of trees. A k forest, denoted by F_k, is a forest consisting of k components and a 1 forest is a tree. A component j is a set $\mathcal{N}_j$ of nodes of G and two different components possess different nodes such that $\mathcal{N}_j \cap \mathcal{N}_l = \varnothing$ for each component j and l of a k forest. A k spanning forest of G is a k forest whose union of components consists of all nodes of G, thus $\cup_{l=1}^{k} \mathcal{N}_l = \mathcal{N}$, and a k spanning forest of G has $N - k$ links. Two k spanning forests are different if they have different sets of links. Finally, we denote by $\gamma(F_k) = \prod_{l=1}^{k} n_l$, where $n_l = |\mathcal{N}_l|$.

Theorem 13 (Matrix Tree Theorem according to Kelmans) *In a graph G with N nodes, the coefficient $(-1)^m c_m(Q)$ of the characteristic polynomial of the Laplacian Q equals, for $m = 0$, $c_0 = 0$ and, for $1 \le m \le N$,*

$$(-1)^m c_m(Q) = \sum_{all\ F_m} \gamma(F_m)$$

where the sum is over all possible m spanning forests of the graph G with precisely m components.

Kelmans Theorem 13 is used in **art.** 87. Kelmans and Chelnokov (1974) also give[3]

$$(-1)^{N-2} c_{N-2}(Q) = 2L^2 - L - \frac{1}{2} \sum_{k=1}^{N} d_k^2$$

$$(-1)^{N-3} c_{N-3}(Q) = \frac{4}{3} L^3 - 2L^2 - (L-1) \sum_{k=1}^{N} d_k^2 + \frac{1}{3} \sum_{k=1}^{N} d_k^3 - 2\blacktriangle_G$$

where $\blacktriangle_G$ is the number of triangles in G. Invoking the Newton identities in **art.** 198, we may verify that these expressions for the coefficients $c_k(Q)$ are consistent with (4.4) and (4.6).

4.1.3 The complexity

82. The *complexity* $\xi(G)$ of the graph G equals the number of all possible spanning trees in the graph. Let J denote the all one matrix with $(J)_{ij} = 1$ and $J = u.u^T$, then

$$\mathrm{adj} Q = \xi(G) J \tag{4.13}$$

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[3] The first result is presented without proof, but a reference to the Russian PhD thesis of Kelmans is given, while the second result is obtained by using special types of graphs.

where $X^{-1} = \frac{\mathrm{adj}X}{\det X}$. Indeed, if $\mathrm{rank}(Q) < N - 1$, then every cofactor of Q is zero, thus $\mathrm{adj}Q = 0$ and (4.13) shows that $\xi(G) = 0$ implying that the graph is disconnected. If $\mathrm{rank}(Q) = N - 1$, then $Q\mathrm{adj}Q = I \det Q = 0$ which means that each column vector of $\mathrm{adj}Q$ is orthogonal to the $N - 1$ dimensional space spanned by the row vectors of Q. Thus, each column vector of $\mathrm{adj}Q$ belongs to the null space or kernel of Q, which is one dimensional and spanned by u, since $Qu = 0$. Hence, each column vector of $\mathrm{adj}Q$ is a multiple of the vector u. Since Q is symmetric, so is $\mathrm{adj}Q$ and all the multipliers must be equal such that $\mathrm{adj}Q = \alpha J$. Since $\mathrm{adj}Q = \det\left((BB^T)_{N-1}\right)$, the Matrix Tree Theorem 12 in **art.** 81 shows that $\xi(G)$ equals the total number of trees that span N nodes.

We apply the relation (4.13) to the complete graph K_N where $Q = NI - J$. Equation (4.13) demonstrates that all elements of $\mathrm{adj}Q$ are equal to $\xi(G)$. Hence, it suffices to compute one suitable element of $\mathrm{adj}Q$, for example, $(\mathrm{adj}Q)_{11}$, which is equal to the determinant of the $(N-1) \times (N-1)$ principal submatrix of Q obtained by deleting the first row and column in Q,

$$(\mathrm{adj}Q)_{11} = \det \begin{bmatrix} N-1 & -1 & \cdots & -1 \\ -1 & N-1 & \cdots & -1 \\ \vdots & & \ddots & \vdots \\ -1 & -1 & \cdots & N-1 \end{bmatrix}$$

Adding all rows to the first and subsequently adding this new first row to all other rows gives

$$(\mathrm{adj}Q)_{11} = \det \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & N & 1 & \cdots & 1 \\ \vdots & & \ddots & \vdots \\ 1 & 1 & \cdots & N & 1 \end{bmatrix} = \det \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & N & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & N \end{bmatrix} = N^{N-2}$$

Hence, the total number of spanning trees in the complete graph K_N, which is also the total number of possible spanning trees in any graph with N nodes, equals N^{N-2}. This is a famous theorem of Cayley of which many proofs exist, see, e.g., Lovász (2003) and van Lint and Wilson (1996, Chapter 2).

83. Equation (4.13) shows that all N minors M_{N-1} of Q are equal to $\xi(G)$. Application of the general relation (8.4) for the coefficients of the characteristic polynomial then gives $c_1 = -N\xi(G)$, as earlier established in **art.** 81. Using (8.8) and the fact that $\mu_N = 0$ (see **art.** 66) yields $c_1 = -\prod_{j=1}^{N-1} \mu_j$. By combining both, the total number of spanning trees $\xi(G)$ in a connected graph is expressed in terms of the eigenvalues of the Laplacian Q as

$$\xi(G) = \frac{1}{N} \prod_{j=1}^{N-1} \mu_j \tag{4.14}$$

84. The complexity of G is also given by

$$\xi\left(G\right) = \frac{\det\left(J + Q\right)}{N^2} \tag{4.15}$$

Indeed, observe that $JQ = \left(JB\right)B^T = 0$ since $JB = 0$ as follows from $J = u.u^T$ and from (2.1) in **art.** 1. Hence,

$$\left(NI - J\right)\left(J + Q\right) = NJ + NQ - J^2 - JQ = NQ$$

and

$$\text{adj}\left(\left(NI - J\right)\left(J + Q\right)\right) = \text{adj}\left(J + Q\right)\text{adj}\left(NI - J\right) = \text{adj}\left(NQ\right)$$

Since $Q_{K_N} = NI - J$ and as shown in **art.** 82, $\text{adj}(NI - J) = N^{N-2}J$ and since $\text{adj}(NQ) = N^{N-1}\text{adj}Q = N^{N-1}\xi\left(G\right)J$, where we have used (4.13),

$$\text{adj}\left(J + Q\right)J = N\xi\left(G\right)J$$

Left multiplication with $J + Q$ taking into account that $JQ = 0$ and $J^2 = NJ$ finally gives

$$\left(J + Q\right)\text{adj}\left(J + Q\right)J = \det\left(J + Q\right)J = N^2\xi\left(G\right)J$$

which proves (4.15).

85. Since $Qu = 0$, we also have that $QJ = O$ and, after taking the transpose, $J^T Q^T = JQ = O$. Hence, the Laplacian $Q = \Delta - A$ commutes with the all one matrix J, $QJ = JQ$. Recall from **art.** 41 that the adjacency matrix A and the all one matrix J only commute if the graph is regular. Since commuting matrices have a common, not necessarily complete set of eigenvectors on Lemma 11, Q and J have a common basis of eigenvectors. The all one vector u is also an eigenvector of J with eigenvalue $\lambda\left(J\right) = N$.

All eigenvalues (5.1) of the rank 1 symmetric matrix $J = u.u^T$ are explicitly known. If X is the matrix containing as columns the eigenvectors $j_1 = u, j_2, \ldots, j_N$ of J and $X^T X = I$, then $\text{diag}(\lambda_k\left(Q\right)) = X^T Q X$. The matrix $Y = I - \frac{1}{N}J$ projects any other vector x orthogonal to the vector u. Hence, a set of eigenvectors of J consists of $N - 1$ columns of Y and the vector u. However, there are infinitely many sets of basisvectors that are also eigenvectors of J, but not necessarily of Q. Hence, the difficulty lies in finding X_Q among all those of X_J.

86. Vice versa, if x_k is an eigenvector of Q belonging to $\mu_k > 0$, then it is also an eigenvector of J because $Jx_k = 0$ for any x_k orthogonal to u. This means that the eigenvalues of $J + Q$ consists of the eigenvalue N with eigenvector u and the set $0 < \mu_j, \mu_{j-1}, \ldots, \mu_1$ where $j \leq N - 1$. If $j = N - 1$, Theorem 11 shows that the graph is connected, else the graph is disconnected. A connected graph satisfies $\det\left(J + Q\right) = N \prod_{j=1}^{N-1} \mu_j$ and the complexity via (4.15) leads again to (4.14).

If G_r is a regular graph where all nodes have degree r, then **art.** 74 shows that

$\mu_j = r - \lambda_{N+1-j}$. Substituted in (4.14) yields

$$\xi(G_r) = N^{-1} \prod_{j=1}^{N-1} (r - \lambda_{N+1-j}) = N^{-1} \prod_{m=2}^{N} (r - \lambda_m)$$

The characteristic polynomial $c_{A_r}(x)$ of the adjacency matrix of G_r equals

$$c_{A_r}(x) = (x - r) \prod_{m=2}^{N} (x - \lambda_m)$$

from which we deduce that

$$\left. \frac{dc_{A_r}(x)}{dx} \right|_{x=r} = \prod_{m=2}^{N} (r - \lambda_m) = N\xi(G_r)$$

87. Since $c_0 = \det Q = 0$, the characteristic polynomial of the Laplacian is

$$c_Q(x) = x \sum_{k=0}^{N-1} c_{k+1}(Q) x^k$$

Applying the Newton equations (**art.** 198) to $\frac{c_Q(x)}{x}$ gives

$$\sum_{k=1}^{N-1} \frac{1}{\mu_k} = -\frac{c_2(Q)}{c_1(Q)}$$

Since all zeros of $\sum_{k=0}^{N-1} c_{k+1}(Q) x^k$ for a connected graph are positive and $\frac{c_{N-1}}{c_N} = -2L$ (**art.** 81), **art.** 198 provides the bound

$$-\frac{c_2(Q)}{c_1(Q)} \geq \frac{(N-1)^2}{2L}$$

Art. 83 shows that $c_1(Q) = -N\xi(G)$, while the Matrix Tree Theorem 12 in **art.** 81 indicates that $c_2(Q)$ equals the number of all spanning trees with $N-2$ links in all subgraphs of G that are obtained after deleting any pair of two nodes in G.

For a tree $G = T$, we have that $\xi(G) = 1$ and $c_1(Q) = -N$, while Kelmans' Theorem 13 states that

$$c_2(Q) = \sum_{\text{all } F_2} \gamma(F_2)$$

where the sum is over all possible 2 spanning forests of the graph G with precisely two components. A 2 spanning forest is constructed from a spanning tree of G in which one link is deleted such that two disjoint trees T_1 and T_2 are obtained. Now, $\gamma(F_2) = n_1 n_2$ is also equal to the number of ways of choosing a node v_1 in tree T_1 (component 1) and a node v_2 in T_2 (component 2). Since G is a tree, the number of pairs (T_1, v_1) and (T_2, v_2) equals the distance $h(v_1, v_2)$ in hops between node v_1

and node v_2, since (T_1, v_1) and (T_2, v_2) can only be obtained by deleting one of the links in G on the path from v_1 to v_2. Thus,

$$c_2\left(Q\right) = \sum_{v_1 \in \mathcal{N}} \sum_{v_2 \neq v_1 \in \mathcal{N}} h\left(v_1, v_2\right) = \frac{N(N-1)}{2} E\left[H_T\right]$$

where H_T is the hopcount in the tree T. Hence, the average hopcount in any tree satisfies

$$E\left[H_T\right] = \frac{2}{N-1} \sum_{k=1}^{N-1} \frac{1}{\mu_k} \tag{4.16}$$

Mohar (1991) has attributed formula (4.16) to Brendan McKay, who provided the above derivation. Section 7.8.3 demonstrates, via inequality (7.26), that the right hand side of (4.16) is a lower bound for the average hopcount in any graph.

4.2 Second smallest eigenvalue of the Laplacian Q

The second smallest eigenvalue μ_{N-1} of the Laplacian has many interesting proper ties and was coined by Fiedler (1973), the algebraic connectivity of a graph. Mainly bounds are presented in this section, whereas **art. 97** provides the major motivation to focus in depth on the algebraic connectivity μ_{N-1}.

4.2.1 Upper bounds for μ_{N-1}

88. The eigenvector belonging to the smallest, zero eigenvalue μ_N is u (**art. 66**). In the terminology of **art. 77** and **art. 241**, any constant function $f\left(x\right) = c$ is an eigenfunction of μ_N. Rayleigh's theorem (**art. 152**) states that, for any function f orthogonal to a constant function c, we have

$$\mu_{N-1}\left(f, f\right) \leq \left(Qf, f\right)$$

and the minimizer, for which equality holds, is the eigenfunction belonging to the second smallest eigenvalue μ_{N-1}. With **art. 77**, we obtain

$$\mu_{N-1} \leq \frac{\sum_{l \in \mathcal{L}} \left(f\left(l^+\right) - f\left(l^-\right)\right)^2}{\sum_{n \in \mathcal{N}} f^2\left(n\right)} \tag{4.17}$$

for any f that satisfies $(f, c) = c \sum_{n \in \mathcal{N}} f\left(n\right) = 0$. The latter condition is always fulfilled if we choose $f\left(x\right) = g\left(x\right) - \frac{1}{N} \sum_{n \in \mathcal{N}} g\left(n\right)$, where the last term can be interpreted as an average of g over all nodes of the graph. In addition, for such a choice, $(f\left(l^+\right) - f\left(l^-\right)) = (g\left(l^+\right) - g\left(l^-\right))$ such that

$$\mu_{N-1} \leq \frac{\sum_{l \in \mathcal{L}} \left(g\left(l^+\right) - g\left(l^-\right)\right)^2}{\sum_{n \in \mathcal{N}} g^2\left(n\right) - \frac{1}{N} \left(\sum_{u \in \mathcal{N}} g\left(u\right)\right)^2}$$

for any non constant function g.

For example, choose the vector or eigenfunction f as $f(u) = 1$, $f(v) = -1$ and $f(n) = 0$ for any node $n \neq v \neq u$. This vector is orthogonal to the constant, $(f, c) = 0$. Inequality (4.17) then gives

$$\mu_{N\ 1} \leq \frac{d_u + d_v}{2}$$

A sharper bound using the same method is obtained in (4.20).

89. There is an alternative representation for (f, f) or for $x^T x = \|x\|_2^2$ due to Fiedler. Since,

$$\sum_{i=1}^{N} \sum_{j=1}^{N} (x_i - x_j)^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i^2 + 2 \sum_{i=1}^{N} x_i \sum_{j=1}^{N} x_j + \sum_{i=1}^{N} \sum_{j=1}^{N} x_j^2$$

$$= 2N x^T x + 2 \left(u^T x\right)^2$$

and since any eigenvector x that does not belong to $\mu_N = 0$ is orthogonal to u, we find that

$$x^T x = \frac{1}{2N} \sum_{i=1}^{N} \sum_{j=1}^{N} (x_i - x_j)^2$$

Thus, if f is the eigenfunction of Q belonging to $\mu_{N\ 1}$, then

$$\mu_{N\ 1} = \frac{2N \sum_{l \in \mathcal{L}} (f(l^+) - f(l^-))^2}{\sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} (f(u) - f(v))^2} \tag{4.18}$$

The numerator and denominator are invariant to the addition of a constant. If f is not the eigenfunction of Q belonging to $\mu_{N\ 1}$, i.e., $f \neq c$, Rayleigh's principle in **art. 152** states that

$$\mu_{N\ 1} \leq \frac{2N \sum_{l \in \mathcal{L}} (f(l^+) - f(l^-))^2}{\sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} (f(u) - f(v))^2} \tag{4.19}$$

The advantage of this inequality is, that explicit orthogonality for f to the constant function c, $(c, f) = 0$, is not required anymore since it is implicitly incorporated into the denominator. For example, choosing now the eigenfunction f as $f(x) = 1_{\{x=w\}}$ leads, with $(f(u) - f(v))^2 = 1_{\{u=w\}} + 1_{\{v=w\}}$ provided $u \neq v$ and

$$\sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} (f(u) - f(v))^2 = \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N} \backslash \{u\}} 1_{\{u=w\}} + \sum_{v \in \mathcal{N}} \sum_{u \in \mathcal{N} \backslash \{v\}} 1_{\{v=w\}}$$

$$= 2 \sum_{u \in \mathcal{N}} 1_{\{u=w\}} \sum_{v \in \mathcal{N} \backslash \{u\}} 1 = 2(N-1)$$

to

$$\mu_{N\ 1} \leq \frac{N}{N-1} d_w$$

Since the inequality holds for any node w, the sharpest bound is reached when

$d_w = d_{\min}$ and we find an inequality for the second smallest eigenvalue of the Laplacian

$$\mu_{N-1} \le \frac{N}{N-1} d_{\min} \tag{4.20}$$

Since equality is attained for the complete graph K_N as shown in Section 5.1, the bound (4.20) is generally the best possible. Recall that this inequality also follows from (8.62) in Fiedler's Theorem 41 for symmetric, positive semidefinite matrices. The bound (4.20) is also derived from the Alon Milman inequality (4.33) as shown in **art.** 97.

90. We apply (4.20) to the complement G^c of a graph G,

$$\mu_{N-1}(Q^c) \le \frac{N}{N-1} d_{\min}(G^c) = \frac{N}{N-1}(N-1-d_{\max}(G))$$

$$= N - \frac{N}{N-1} d_{\max}(G)$$

Using (4.9) yields a lower bound for the largest eigenvalue of the Laplacian

$$\frac{N}{N-1} d_{\max} \le \mu_1 \le \min(N, 2d_{\max}) \tag{4.21}$$

where the upperbound follows from (4.10).

Grone and Merris (1994) succeeded in improving Fiedler's lower bound (4.21). Since their proof is not illuminating, however, we merely quote the improved lower bound,

$$\mu_1 \ge d_{\max} + 1 \tag{4.22}$$

which they claim is a strict inequality when $d_{\max} < N - 1$. Applying (4.22) to the complement G^c then shows that

$$\mu_1(Q^c) \ge d_{\max}(G^c) + 1 = N - d_{\min}(G)$$

and, with (4.9), that

$$\mu_{N-1}(Q) \le d_{\min}(G) \tag{4.23}$$

4.2.2 Lower bounds for μ_{N-1}

91. *Lower bounds for any Laplacian eigenvalue.* Recently, Bouwer and Haemers (2008) have impressively extended the type of lower bound (4.22) of Grone and Merris.

Theorem 14 (Brouwer and Haemers) *For any graph but $K_m + (N-m)K_1$, the disjoint union of the complete graph K_m and $N - m$ isolated nodes, the j th largest Laplacian eigenvalue is lower bounded, for $1 \le j \le N$, by*

$$\mu_j \ge d_{(j)} - j + 2 \tag{4.24}$$

where $d_{(j)}$ is the j th largest nodal degree.

Proof: The proof of Bouwer and Haemers (2008) cleverly combines the gener alized interlacing Theorem 43 applied to a specific quotient matrix K_π, defined in **art.** 15. The proof is rather complex and thus omitted. $\qquad\square$

Bouwer and Haemers (2008) also discuss graphs for which equality in (4.24) is reached. Since $\mu_j \geq 0$, the bound (4.24) becomes useless when $d_{(j)} < j - 2$.

In fact, we may introduce slack variables $\epsilon_j \geq 0$ in (4.24) to obtain the equality

$$\mu_j = d_{(j)} - j + 2 + \epsilon_j$$

Substitution into the m th moment formula (4.7) specifies the moments $\sum_{j=1}^{N} \epsilon_j^m$. For example, for $m = 1$, we find from (4.2), using $\sum_{j=1}^{N} d_{(j)} = \sum_{j=1}^{N} d_j$,

$$\sum_{j=1}^{N} \epsilon_j = \frac{N(N-3)}{2}$$

which shows that the average of the ϵ_j's increases linearly with N. The cases for higher values of m are more involved, as illustrated for $m = 2$, which is derived from (4.4),

$$\sum_{j=1}^{N} \epsilon_j^2 = \frac{N(2N^2 - 9N + 13)}{6} + 2L + 2\sum_{j=1}^{N} d_j^2 + 2\sum_{j=1}^{N} j(\mu_j - d_j) - 2\sum_{j=1}^{N} d_j \mu_j$$

The last sum is related to the covariance $E[D\mu] - E[D]E[\mu]$ and, in general, difficult to assess. The above method of equating moments (see also **art.** 246) suggests to consider $\mu_j = d_{(j)} + \tilde{\epsilon}_j$, where the difference $\tilde{\epsilon}_j$ can be negative as well as positive, but the average difference is zero.

92. *Lower bounds for μ_{N-1}.* First, the upperbound (4.10) applied to the comple ment G^c,

$$\mu_1(Q^c) \leq 2d_{\max}(G^c) = 2(N - 1 - d_{\min}(G)),$$

and (4.9) give

$$-N + 2 + 2d_{\min}(G) \leq \mu_{N-1}$$

which is, in most cases, useless if the left hand side is negative. Hence, more ingenious methods are needed.

We will now apply the functional framework of **art.** 77 and **art.** 88 to derive a better lower bound for the second smallest eigenvalue of the Laplacian. Assume that f is the eigenfunction of Q belonging to μ_{N-1} for which the equality sign holds in (4.17),

$$\mu_{N-1} = \frac{\sum_{l \in \mathcal{L}} (f(l^+) - f(l^-))^2}{\sum_{n \in \mathcal{N}} f^2(n)}$$

Let node u for which $|f(u)| = \max_{n \in \mathcal{N}} |f(n)| > 0$. Clearly,

$$\sum_{n \in \mathcal{N}} f^2(n) \leq N f^2(u)$$

Since $\sum_{n \in \mathcal{N}} f(n) = 0$ as shown in **art.** 88, there exists a node v for which $f(u) f(v) < 0$. Since $\mu_{N-1} > 0$ provided the graph is connected, it means that there exists a path $\mathcal{P}(v, u)$ from v to u with hopcount $h(\mathcal{P})$. The minimum number of links to connect a graph occurs in a minimum spanning tree (MST) consisting of $N - 1$ links. Only if the diameter $\rho \geq h(\mathcal{P})$ of G is smaller than $N - 1$, we have a strict inequality in

$$\sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-) \right)^2 \geq \sum_{l \in \text{MST}} \left(f(l^+) - f(l^-) \right)^2 \geq \sum_{l \in \mathcal{P}(v,u)} \left(f(l^+) - f(l^-) \right)^2$$

By the Cauchy Schwarz inequality (8.41), we have

$$h(\mathcal{P}) \sum_{l \in \mathcal{P}(v,u)} \left(f(l^+) - f(l^-) \right)^2 \geq \left(\sum_{l \in \mathcal{P}(v,u)} \left| f(l^+) - f(l^-) \right| \right)^2$$

$$\geq \left(\sum_{l \in \mathcal{P}(v,u)} \left(f(l^+) - f(l^-) \right) \right)^2$$

$$= (f(v) - f(u))^2$$

$$\geq f^2(u)$$

because $f(u) f(v) < 0$. Thus,

$$\sum_{l \in \mathcal{P}(v,u)} \left(f(l^+) - f(l^-) \right)^2 \geq \frac{f^2(u)}{h(\mathcal{P})} \geq \frac{f^2(u)}{\rho}$$

Combining all inequalities leads to

$$\mu_{N-1} \geq \frac{1}{\rho N}$$

This bound can only be improved a little by using the definition (4.18). Indeed, using the above inequality based on the Cauchy Schwarz inequality, we have

$$\sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} (f(u) - f(v))^2 \leq \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h(\mathcal{P}(v, u)) \sum_{l \in \mathcal{P}(v,u)} \left(f(l^+) - f(l^-) \right)^2$$

$$= \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h(\mathcal{P}(v, u)) \sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-) \right)^2 1_{\{l \in \mathcal{P}(v,u)\}}$$

$$= \sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-) \right)^2 \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h(\mathcal{P}(v, u)) 1_{\{l \in \mathcal{P}(v,u)\}}$$

$$\leq \rho \sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-) \right)^2 \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} 1_{\{l \in \mathcal{P}(v,u)\}}$$

where the betweenness of a link l is defined as

$$B_l = \frac{1}{2} \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} 1_{\{l \in \mathcal{P}(v,u)\}}$$

Art. 53 shows that the number of links in the union of all shortest hop paths between a same source u and destination v is at most $\left[\frac{N^2}{4}\right]$. This means that an arbitrary link l can only occur in at most $\left[\frac{N^2}{4}\right]$ unions[4] of shortest hop paths between all pairs (u, v),

$$2B_l = \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} 1_{\{l \in \mathcal{P}(v,u)\}} \leq 2 \left[\frac{N^2}{4}\right] \tag{4.25}$$

Thus, (4.18) leads to

$$\mu_{N-1} \geq \frac{4}{\rho N} \tag{4.26}$$

This lower bound (4.26) is the best possible. As mentioned by Mohar (1991), McKay has shown that in a tree of diameter $\rho = t + 2$, obtained from a t hop path, where k nodes are connected to each of its end nodes such that $N = t + 1 + 2k$, (4.26) is sharp if $\frac{k}{t} \to \infty$.

93. We present another interpretation, deduced from **art.** 92, by rewriting

$$r = \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h\left(\mathcal{P}(v,u)\right) 1_{\{l \in \mathcal{P}(v,u)\}}$$

$$= \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h\left(\mathcal{P}(v,u)\right) \left(1_{\{l \in \mathcal{P}(v,u)\}} - 1 + 1\right)$$

$$= \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h\left(\mathcal{P}(v,u)\right) - \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}\backslash\{u\}} h\left(\mathcal{P}(v,u)\right) \left(1 - 1_{\{l \in \mathcal{P}(v,u)\}}\right)$$

because $h\left(\mathcal{P}(u,u)\right) = 0$. In all other cases where nodes u and v are different, $h\left(\mathcal{P}(v,u)\right) \geq 1$, such that the last sum is bounded:

$$\widetilde{r} = \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}\backslash\{u\}} h\left(\mathcal{P}(v,u)\right) \left(1 - 1_{\{l \in \mathcal{P}(v,u)\}}\right)$$

$$\geq \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}\backslash\{u\}} \left(1 - 1_{\{l \in \mathcal{P}(v,u)\}}\right) = 2\binom{N}{2} - \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}\backslash\{u\}} 1_{\{l \in \mathcal{P}(v,u)\}}$$

$$\geq 2\binom{N}{2} - 2\frac{N^2}{4} = \frac{N(N-2)}{2}$$

where in the last line (4.25) has been used. With the definition of the average hopcount,

$$\sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} h\left(\mathcal{P}(v,u)\right) = N\left(N-1\right) E\left[H\right]$$

---

[4] The maximum betweenness in any graph, $B_l \leq \left[\frac{N^2}{4}\right]$, can also be proved differently, as shown by Wang *et al.* (2008).

we thus find

$$\sum_{u\in\mathcal{N}}\sum_{v\in\mathcal{N}} h\left(\mathcal{P}\left(v,u\right)\right) 1_{\{l\in\mathcal{P}(v,u)\}} \le N\left(N-1\right) E\left[H\right] - \frac{N(N-2)}{2}$$

Again, (4.18) shows that

$$\mu_{N\;1} \ge \frac{2}{\left(N-1\right) E\left[H\right] - \frac{(N\;2)}{2}}$$

or

$$E\left[H\right] \ge \frac{2}{\left(N-1\right)\mu_{N\;1}} + \frac{\left(N-2\right)}{2\left(N-1\right)}$$

94. *Another type lower bounds for $\mu_{N\;1}$.* Let f be the eigenfunction of Q belonging to $\mu_{N\;1}$. Since f is non zero and orthogonal to the constant function,

$$0 = \sum_{n\in\mathcal{N}} f\left(n\right) = \sum_{n^+\in\mathcal{N}} f\left(n^+\right) - \sum_{n\;\in\mathcal{N}} \left|f\left(n\;\right)\right|$$

where, for $n^+ \in \mathcal{N}$, $f\left(n^+\right) > 0$ and $n\;\in \mathcal{N}$, $f\left(n\;\right) \le 0$. Let us define the set of positive nodes $\mathcal{N}^+ = \{n \in \mathcal{N} : f\left(n\right) > 0\}$ and $\mathcal{N}\;= \mathcal{N}\backslash\mathcal{N}^+$. Similarly, let $\mathcal{L}^+ = \{u^+v^+ \in \mathcal{N}: u^+, v^+ \in \mathcal{N}^+\}$ denote the set of all links between positive nodes and $\mathcal{L}\;= \{u^+v\;\in \mathcal{N}: u^+ \in \mathcal{N}^+, v\;\in \mathcal{N}\;\}$ denote the set of all links between positive nodes and negative nodes. Since f is an eigenfunction of Q, for each nodal component $u \in \mathcal{N}$ holds that

$$\left(Qf\right)\left(u\right) = \mu_{N\;1} f\left(u\right)$$

Multiplying both sides by $f\left(u\right)$ and summing over positive nodes yields

$$\mu_{N\;1} = \frac{\sum_{v\in\mathcal{N}^+} Qf\left(v\right) f\left(v\right)}{\sum_{v\in\mathcal{N}^+} f^2\left(v\right)}$$

Using the definition (**art.** 2) of the Laplacian $Q = \Delta - A$,

$$\sum_{v\in\mathcal{N}^+} Qf\left(v\right) f\left(v\right) = \sum_{v\in\mathcal{N}^+} f\left(v\right)\left(\Delta f - Af\right)\left(v\right)$$

$$= \sum_{v\in\mathcal{N}^+} f\left(v\right)\left(d\left(v\right) f\left(v\right) - \sum_{u\in\text{neighbor}(v)} f\left(u\right)\right)$$

$$= \sum_{v\in\mathcal{N}^+}\sum_{u\in\text{neighbor}(v)} f\left(v\right)\left(f\left(v\right) - f\left(u\right)\right)$$

Further, after splitting the neighbors into positive and negative nodes,

$$\sum_{v\in\mathcal{N}^+} Qf\left(v\right) f\left(v\right) = \sum_{v^+u^+\in\mathcal{L}^+} f\left(v\right)\left(f\left(v\right) - f\left(u\right)\right) + \sum_{v^+u\;\in\mathcal{L}} f\left(v\right)\left(f\left(v\right) - f\left(u\right)\right)$$

Since the graph is bidirectional, i.e., $A^T = A$, the link $v^+u^+ = u^+v^+$ appears twice in the sum such that

$$\sum_{v^+u^+ \in \mathcal{L}^+} f(v)(f(v) - f(u)) = \sum_{u^+v^+ \in \mathcal{L}^+} \{f(v)(f(v) - f(u)) + f(u)(f(u) - f(v))\}$$

$$= \sum_{u^+v^+ \in \mathcal{L}^+} (f(v) - f(u))^2$$

where a link $u^+v^+ \in \mathcal{L}^+$ is only counted once. Similarly as before, we denote the link $l = u^+v^+$ by the head of link as $l^+ = u^+$ and by the tail as $l^- = v^+$. Thus, we arrive at

$$\sum_{v \in \mathcal{N}^+} Qf(v) f(v) = \sum_{l \in \mathcal{L}^+} (f(l^+) - f(l^-))^2 + \sum_{v^+u^- \in \mathcal{L}} f(v)(f(v) - f(u))$$

and

$$\mu_{N-1} = \frac{\sum_{l \in \mathcal{L}^+} (f(l^+) - f(l^-))^2 + \sum_{v^+u^- \in \mathcal{L}} f(v)(f(v) - f(u))}{\sum_{v \in \mathcal{N}^+} f^2(v)}$$

Also the last sum in the numerator is non negative because each term

$$f(v^+)(f(v^+) - f(u^-)) > 0$$

such that

$$\sum_{v \in \mathcal{N}^+} Qf(v) f(v) \geq \sum_{u^+v^+ \in \mathcal{L}^+} (f(v) - f(u))^2$$

which leads to a lower bound

$$\mu_{N-1} \geq \frac{\sum_{l \in \mathcal{L}^+} (f(l^+) - f(l^-))^2}{\sum_{n \in \mathcal{N}^+} f^2(n)} \tag{4.27}$$

The lower bound (4.27) resembles the upper bound (4.17), except that only positive nodes and links are considered and that f is not arbitrary, but the eigenfunction of Q belonging to the eigenvalue μ_{N-1}.

We can improve this lower bound (4.27) by incorporating positive terms in $\sum_{v^+u^- \in \mathcal{L}} f(v)(f(v) - f(u))$, that we have neglected. This means that also links outside the positive cluster are taken into account. Following Alon (1986), we can define $g(v) = f(v) 1_{\{v \in \mathcal{N}^+\}}$ such that

$$\sum_{v^+u^- \in \mathcal{L}} f(v)(f(v) - f(u)) \geq \sum_{v^+u^- \in \mathcal{L}} (g(v) - g(u))^2$$

With this function, the first sum remains unaltered,

$$\sum_{l \in \mathcal{L}^+} (f(l^+) - f(l^-))^2 = \sum_{l \in \mathcal{L}^+} (g(l^+) - g(l^-))^2 = \sum_{l \in \mathcal{L}} (g(l^+) - g(l^-))^2$$

and, also $\sum_{n\in\mathcal{N}+} f^2(n) = \sum_{n\in\mathcal{N}+} g^2(n) = \sum_{n\in\mathcal{N}} g^2(n)$. Thus, the improved lower bound is

$$\mu_{N\ 1} \geq \frac{\sum_{l\in\mathcal{L}}(g(l^+) - g(l^-))^2}{\sum_{n\in\mathcal{N}} g^2(n)} \tag{4.28}$$

95. Let $G + \{e\}$ denote a graph obtained from G by adding a link e between two nodes of G. For any f orthogonal to a constant function, we have that

$$\frac{\sum_{l\in\mathcal{L}(G+\{e\})}(f(l^+) - f(l^-))^2}{\sum_{n\in\mathcal{N}} f^2(n)} = \frac{\sum_{l\in\mathcal{L}(G)}(f(l^+) - f(l^-))^2}{\sum_{n\in\mathcal{N}} f^2(n)} + \frac{(f(e^+) - f(e^-))^2}{\sum_{n\in\mathcal{N}} f^2(n)}$$

If $f = f_{G+\{e\}}$ is an eigenfunction of $G + \{e\}$ corresponding to $\mu_{N\ 1}(G + \{e\})$, then (4.17) shows that

$$\mu_{N\ 1}(G + \{e\}) \leq \mu_{N\ 1}(G) + \frac{(f_{G+\{e\}}(e^+) - f_{G+\{e\}}(e^-))^2}{\sum_{n\in\mathcal{N}} f^2_{G+\{e\}}(n)}$$

On the other hand, if $f = f_G$ is an eigenfunction of G corresponding to $\mu_{N\ 1}(G)$, then

$$\mu_{N\ 1}(G + \{e\}) \geq \mu_{N\ 1}(G) + \frac{(f_G(e^+) - f_G(e^-))^2}{\sum_{n\in\mathcal{N}} f^2_G(n)}$$

In the first bound,

$$b = \frac{(f_{G+\{e\}}(e^+) - f_{G+\{e\}}(e^-))^2}{\sum_{n\in\mathcal{N}} f^2_{G+\{e\}}(n)}$$

$$= \frac{f^2_{G+\{e\}}(e^+) + f^2_{G+\{e\}}(e^-) - 2f_{G+\{e\}}(e^+)f_{G+\{e\}}(e^-)}{f^2_{G+\{e\}}(e^+) + f^2_{G+\{e\}}(e^-) + \sum_{n\in\mathcal{N}\backslash\{e^+,e^-\}} f^2_{G+\{e\}}(n)}$$

$$\leq \frac{f^2_{G+\{e\}}(e^+) + f^2_{G+\{e\}}(e^-) + 2|f_{G+\{e\}}(e^+)||f_{G+\{e\}}(e^-)|}{f^2_{G+\{e\}}(e^+) + f^2_{G+\{e\}}(e^-)}$$

$$\leq 2$$

because $\max_{x\geq 0, y\geq 0} \frac{2xy}{x^2+y^2} = \max_{r=\frac{y}{x}\geq 0} \frac{2r}{1+r^2} = 1$. With $\frac{(f_G(e^+) - f_G(e^-))^2}{\sum_{n\in\mathcal{N}} f^2_G(n)} \geq 0$ in the second bound, we arrive at

$$\mu_{N\ 1}(G) \leq \mu_{N\ 1}(G + \{e\}) \leq \mu_{N\ 1}(G) + 2 \tag{4.29}$$

The same bounds (4.29) are elegantly proved by invoking interlacing (**art. 183**) on $Q_{G+\{e\}} = Q_G + Q_{\{e\}}$. Indeed, the Laplacian $Q_{\{e_{ij}\}}$ of a link e_{ij} between node i and j has precisely four non zero elements: $q_{ij} = q_{ji} = -1$ and $q_{ii} = q_{jj} = 1$. The eigenvalues of $Q_{\{e_{ij}\}}$ are obtained from $\det(Q_{\{e\}} - \mu I)$ after expanding the determinant in cofactors over row i (or j),

$$\det(Q_{\{e\}} - \mu I) = (-1)^{2i}(-\mu)^{N-2}(1-\mu)^2 - (-1)^{i+j}(-1)^{j+i}(-\mu)^{N-2}$$

$$= (-\mu)^{N-1}(\mu - 2)$$

The eigenvalues of $Q_{\{e_{ij}\}}$ are thus $[0]^{N\ 1}$ and 2; the interlacing inequality (8.72) leads to (4.29).

Art. 69 shows that, by adding one link, the sum of all eigenvalues increases by 2. Hence, when the upper bound in (4.29) is achieved, all other eigenvalues of $Q_{G+\{e\}}$ are precisely equal to those of Q_G.

4.3 Partitioning of a graph

The problem of graph partitioning consists of dividing the nodes of a graph into a number of disjoint groups, also called partitions (see **art.** 14), such that a certain criterion is met. The most popular criterion is that the number of links between these disjoint groups is minimized. Sometimes, the number of those partitions and their individual size is prescribed. Most, but not all (see **art.** 96), variants of the graph partitioning problem are NP hard.

96. *Graph partitioning into two disjoint subsets.* When confining to a graph parti tioning into two disjoint subsets (subgroups, clusters, partitions,...), an index vector y can be defined with vector component $y_j = 1$ if the node j belongs to one par tition and $y_j = -1$ if node j belongs to the other partition. The number of links R between the two disjoint subsets, also called the cut size or size of the separator, elegantly follows from the characteristic property (4.11) of the Laplacian,

$$R = \frac{1}{4}\sum_{l\in\mathcal{L}}(y_{l^+} - y_{l^-})^2 = \frac{1}{4}y^T Q y \tag{4.30}$$

because, only if the starting node l^+ and the ending node l^- of a link l belong to a different partition, $(y_{l^+} - y_{l^-})^2 = 4$, else $y_{l^+} = y_{l^-}$. The minimum cut size is obviously

$$R_{\min} = \min_{y\in\mathbb{Y}}\frac{1}{4}y^T Q y$$

where $\mathbb{Y}$ is the set of all possible index vectors of the N dimensional space with either -1 or 1 components.

Since all eigenvectors $\{x_k\}_{1\leq k\leq N}$ of the Laplacian Q are orthogonal (**art.** 151), any vector can be written as a linear combination. Let $y = \sum_{j=1}^{N}\alpha_j x_j$, then

$$R = \frac{1}{4}\sum_{j=1}^{N}\alpha_j\sum_{k=1}^{N}\alpha_k x_j^T Q x_k$$

and using the orthogonality property (8.25) in **art.** 151, we obtain

$$R = \frac{1}{4}\sum_{j=1}^{N}\alpha_j^2\mu_j \tag{4.31}$$

Since $\mu_N = 0$ and all other eigenvalues are larger than zero for a connected graph

(Theorem 10), the alternative eigenvalue expression (4.31) shows that R is a sum of positive real numbers.

Although Stoer and Wagner (1997) have presented a highly efficient, non spectral min cut algorithm with a computational complexity of $O\left(NL + N^2 \log N\right)$, which demonstrates that the min cut problem is not NP hard, the minimization of (4.31) is generally difficult. However, if one chooses in (4.30) $y = \alpha_{N-1} x_{N-1}$, then $R = \frac{1}{4}\alpha_{N-1}^2 \mu_{N-1}$, which is, in view of (4.31), obviously the best possible to minimize R. Unfortunately, choosing the index vector y parallel to the Fiedler vector x_{N-1} is generally not possible, because $x_{N-1} \notin \mathbb{Y}$. A good strategy is to choose the sign of the components in y according to the sign of the corresponding component in the Fiedler vector. A slightly better approach is the choice $y = \alpha_N u + x_{N-1}$, since the eigenvector u belonging to $\mu_N = 0$ does not affect the value of R in (4.31) and it provides a higher degree of freedom to choose the size of each partition. This strategy agrees with Fiedler's graph partitioning explained in **art. 103**.

97. *The Alon Milman inequality.* Another approach to the separator problem is to establish useful bounds. As we will demonstrate here, it turns out that the algebraic connectivity μ_{N-1} plays an important role in such bounds. Our starting point is the upper bound in (4.17) for μ_{N-1}. The ingenuity lies in finding a function f, introduced in **art. 88**, satisfying $(f, c) = 0$ that has both a graph interpretation and that provides a tight bound for μ_{N-1} in (4.17). Alon and Milman (1985) have proposed the function

$$g\left(u\right) = \frac{1}{a} - \left(\frac{1}{a} + \frac{1}{b}\right)\frac{\min\left(h, h\left(u, A\right)\right)}{h}$$

where $(g, c) \neq 0$ such that $f = g - \overline{g}$ in **art. 88**, with $\overline{g} = \frac{1}{N}\sum_{n \in \mathcal{N}} g\left(n\right)$. Further, h is the distance (in hops) between two disjoint subsets A and B of $\mathcal{N}$, $h\left(u, A\right)$ is the shortest distance of node $u \in \mathcal{N}$ to a node of the set A and $a = \frac{N_A}{N}$ and $b = \frac{N_B}{N}$, where $N_k = |\mathcal{N}_k|$ is the number of nodes of set $\mathcal{N}_k$. Clearly, if $u \in A$, then $g\left(u\right) = \frac{1}{a}$, while, if $u \in B$, then $h\left(u, A\right) = h$ and $g\left(u\right) = -\frac{1}{b}$. Moreover, if u and v are adjacent, i.e., they are either head $(u = l^+)$ or tail $(u = l^-)$ of a link l, then

$$\left|g\left(u\right) - g\left(v\right)\right| \leq \frac{1}{h}\left(\frac{1}{a} + \frac{1}{b}\right) \tag{4.32}$$

Indeed, if u and v belong to the same set, then $g\left(u\right) - g\left(v\right) = 0$. If $u \in A$ and $v \notin A$, then $h\left(v, A\right) = 1$, because u and v are adjacent and $g\left(u\right) - g\left(v\right) = \left(\frac{1}{a} + \frac{1}{b}\right)\frac{1}{h}$. If both u and v do not belong to A, then $\left|h\left(v, A\right) - h\left(u, A\right)\right| \leq 1$ and

$$\left|g\left(u\right) - g\left(v\right)\right| = \frac{1}{h}\left(\frac{1}{a} + \frac{1}{b}\right)\left|-\min\left(h, h\left(u, A\right)\right) + \min\left(h, h\left(v, A\right)\right)\right|$$

where the difference of the min operator is largest and equal to 1 if not both $h(u, A)$ and $h\left(v, A\right)$ are larger than h. This proves (4.32). Hence, using this bound (4.32),

the numerator in (4.17) is

$$\sum_{l \in \mathcal{L}} \left(f\left(l^+\right) - f\left(l^-\right) \right)^2 = \sum_{l \in \mathcal{L}} \left(g\left(l^+\right) - g\left(l^-\right) \right)^2 = \sum_{l \in \mathcal{L} \setminus \{A \cup B\}} \left(g\left(l^+\right) - g\left(l^-\right) \right)^2$$

$$\leq \frac{1}{h^2} \left(\frac{1}{a} + \frac{1}{b} \right)^2 (L - L_A - L_B)$$

where L_A and L_B are the number of links in the sets A and B respectively. The denominator of (4.17) is

$$\sum_{n \in \mathcal{N}} f^2(n) \geq \sum_{n \in (A \cup B)} f^2(n) = \sum_{n \in A} \left(g(n) - g \right)^2 + \sum_{n \in B} \left(g(n) - g \right)^2$$

$$= N_A \left(\frac{1}{a} - g \right)^2 + N_B \left(\frac{1}{b} + g \right)^2$$

$$= N \left(\frac{1}{a} + \frac{1}{b} + (a+b) g^2 \right) \geq N \left(\frac{1}{a} + \frac{1}{b} \right)$$

Finally, with (4.17), Alon and Milman (1985) arrive at

$$\mu_{N-1} \leq \frac{1}{Nh^2} \left(\frac{1}{a} + \frac{1}{b} \right) (L - L_A - L_B) = \frac{1}{h^2} \left(\frac{1}{N_A} + \frac{1}{N_B} \right) (L - L_A - L_B) \tag{4.33}$$

The Alon Milman inequality (4.33) shows that a large algebraic connectivity μ_{N-1} leads to a high number of links between the two clusters A and B. Indeed, consider all subsets A and B in a graph G with a fixed number of nodes N_A and N_B and same separation h, then a large μ_{N-1} implies a large number of links $L - L_A - L_B$ between any pair — thus also minimal pairs — of subsets A and B. Hence, a large μ_{N-1} means a higher inter twined subgraph structure and, consequently, it is more difficult to cut away a subgraph from G. A graph with large second smallest Laplacian eigenvalue μ_{N-1} is thus more "robust", in the sense of being better connected or interlinked. Just this property of μ_{N-1} has made the second smallest Laplacian eigenvalue a fundamental characterizer of the robustness of a graph.

However, the algebraic connectivity μ_{N-1} should not be viewed as a strict dis connectivity or robustness metric. Fig. 4.1 depicts two graphs G_1 and G_2, each with $N = 7$ nodes, $L = 10$ links and diameter $\rho = 4$, but with different al gebraic connectivity $\mu_{N-1}(G_1) = 0.6338$ and $\mu_{N-1}(G_2) = 0.5858$. Although $\mu_{N-1}(G_1) > \mu_{N-1}(G_2)$, it is easier to disconnect G_1 than G_2, because one link removal disconnects G_1, while two links need to be deleted in G_2.

98. *Bounds for the separator.* The Alon Milman method of **art.** 97 can be extended to deduce bounds for the separator S of two disjoint subsets A and B, that are at a distance h from each other. The separator S is the set of nodes at a distance less than h hops from A and not belonging to A nor B,

$$S = \{ u \in \mathcal{N} \setminus A : h(u, A) < h \}$$

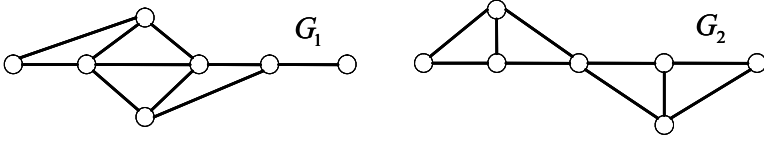and $A \cup B \cup S = \mathcal{N}$. Sometimes, when $h = 1$, the separator is called the cut size,

Fig. 4.1. Two graphs G_1 and G_2, each with $N = 7$ nodes, $L = 10$ links and diameter $\rho = 4$, but with different algebraic connectivity.

since there is a cut that splits the graph into two partitions. As in **art. 97**, we define $a = \frac{N_A}{N}$, $b = \frac{N_B}{N}$ and $s = \frac{N_S}{N}$, where N_C is the number of nodes in the set C. Instead of using the inequality (4.17), Pothen *et al.* (1990) start from the Fiedler inequality (4.19) in which they use

$$f(u) = 1 - \frac{2}{h} \min(h, h(u, A))$$

that is recognized as the Alon Milman function $g(u)$ with $a = b = 1$. If $u \in S$, then $f(u) = 1 - \frac{2}{h}h(u, A)$ and $1 - \frac{2}{h} \geq f(u) \geq 1 - \frac{2(h\ 1)}{h} = -\left(1 - \frac{2}{h}\right)$. The numerator in (4.19) is computed precisely as in **art. 97** with $a = b = 1$,

$$\sum_{l \in \mathcal{L}} \left(f(l^+) - f(l^-)\right)^2 \leq \left(\frac{2}{h}\right)^2 (L - L_A - L_B)$$

$$\leq \left(\frac{2}{h}\right)^2 s N d_{\max}$$

The denominator n in (4.19) is

$$n = \frac{1}{2} \sum_{u \in \mathcal{N}} \sum_{v \in \mathcal{N}} (f(u) - f(v))^2$$

$$= \left(\sum_{u \in A} \sum_{v \in S} + \sum_{u \in A} \sum_{v \in B} + \sum_{u \in B} \sum_{v \in S} + \sum_{u \in S} \sum_{v \in S : v > u}\right) (f(u) - f(v))^2$$

$$\geq \left(\sum_{u \in A} \sum_{v \in S} + \sum_{u \in A} \sum_{v \in B} + \sum_{u \in B} \sum_{v \in S}\right) (f(u) - f(v))^2$$

$$\geq \left(1 - \left(1 - \frac{2}{h}\right)\right)^2 N^2 as + (1 - (-1))^2 N^2 ab + \left(-1 + \left(1 - \frac{2}{h}\right)\right)^2 N^2 bs$$

$$= \left(\frac{2}{h}\right)^2 N^2 \{s(a + b) + h^2 ab\}$$

With $b = 1 - a - s$, we arrive at

$$\mu_{N\ 1} \leq \frac{s d_{\max}}{s(1 - s) + a(1 - a - s)h^2} \tag{4.34}$$

which provides a quadratic inequality in s, from which a lower bound for s can be derived.

99. Pothen *et al.* (1990) present another inequality for the normalized size s of the separator, that is a direct application of the Wielandt Hoffman inequality (8.75) for symmetric matrices. We can always relabel the nodes in the graph G corresponding to the sets A, B and S such that the Laplacian becomes

$$
Q = \left[\begin{array}{ccc}
Q_{Na\times Na} & O_{Na\times Nb} & Q_{Na\times Ns} \\
O_{Nb\times Na} & Q_{Nb\times Nb} & Q_{Nb\times Ns} \\
(Q_{Na\times Ns})^T & (Q_{Nb\times Ns})^T & Q_{Ns\times Ns}
\end{array} \right]
$$

The idea, then, is to consider another matrix, whose eigenvalues are all known, such as $M = \text{diag}(J_{Na\times Na}, J_{Nb\times Nb}, J_{Ns\times Ns})$, where J is the all one matrix. The eigenvalues of M are those of the separate block matrices, that follow from (5.1) as Na, Nb, Nc and all the others are zero. Let us assume that $a \geq b \geq c$. We apply the Wielandt Hoffman inequality (8.75) to M and $-Q$ (to have consistent ordering in the eigenvalues) such that

$$
\sum_{k=1}^{n} \lambda_k(-Q)\,\lambda_k(M) = -\sum_{k=1}^{n} \mu_{N+1\ k}\lambda_k(M) = -\left(0.Na + \mu_{N\ 1}Nb + \mu_{N\ 2}Ns\right)
$$

while $\text{trace}(-QM) = -\text{trace}(QM)$ and, with the shorter notation for the square matrix $R_{Nl\times Nl} = R_{Nl}$,

$$
\text{trace}(QM) = \text{trace}(Q_{Na}J_{Na}) + \text{trace}(Q_{Nb}J_{Nb}) + \text{trace}(Q_{Ns}J_{Ns})
$$

$$
= \left(\sum_{u\in A} + \sum_{u\in B} + \sum_{u\in S} \right)(d_u - d_u^*)
$$

$$
= 2\left(L - L_A - L_B - L_S\right)
$$

where d_u^* is the number of links incident to the node u and with end node in the same set as u. Substituting both in (8.75) yields

$$
\mu_{N\ 1}Nb + \mu_{N\ 2}Ns \leq 2\left(L - L_A - L_B - L_S\right)
$$
$$
\leq 2\left(L - L_A - L_B\right) \leq 2Nsd_{\max}
$$

from which, using $b = 1 - a - s$, a lower bound for the size of the separator follows as

$$
s \geq \frac{(1-a)\,\mu_{N\ 1}}{2d_{\max} - (\mu_{N\ 2} - \mu_{N\ 1})}
$$

This inequality, that contains beside the algebraic connectivity $\mu_{N\ 1}$ also the gap $\mu_{N\ 2} - \mu_{N\ 1}$, complements the inequality (4.34).

100. *Applications of the Alon Milman bound (4.33).* Alon and Milman (1985) mention the following applications of the bound (4.33).

First, let $A = \{u\}$ and $B = \mathcal{N}\setminus\{u\}$, then $h = 1$ and $L - L_A - L_B = d_u$, the degree of node u. Since this inequality holds for any node u, the tightest bound is obtained by choosing a node u with minimum degree $d_{\min} = \min_{u\in\mathcal{N}} d_u$, which leads again to (4.20).

Second, let $a = b = \frac{1}{2}$, then the set of all links connecting a node in A to a node in B is called the bisector of G. The minimum number of the bisector is related to min cut, max flow problems. The Alon Milman bound (4.33) shows a lower bound for the bisector,

$$\frac{N}{4}\mu_{N-1} \leq \text{ bisector }(G)$$

Third, if $h > 1$, then every link in the set $\mathcal{L}\backslash(\mathcal{L}_A\cup\mathcal{L}_B)$ is incident with at least one of the $N-N_A-N_B$ nodes of the set $S = \mathcal{N}\backslash(\mathcal{N}_A\cup\mathcal{N}_B)$, such that $L-L_A-L_B \leq (N - N_A - N_B)\,d_{\max}$. The Alon Milman bound (4.33) becomes, using $a + b < 1$,

$$\mu_{N-1} \leq \frac{1}{h^2}\left(\frac{1}{a} + \frac{1}{b}\right)(1 - a - b)\,d_{\max} \leq \frac{1}{abh^2}(1 - a - b)\,d_{\max}$$

$$= \frac{sd_{\max}}{a(1 - a - s)\,h^2}$$

which is clearly weaker than (4.34) because $0 < s < 1$. It provides a lower bound for the fraction $b = \frac{N_B}{N}$ as

$$b \leq \frac{1 - a}{1 + \frac{ah^2\mu_{N-1}}{d_{\max}}} \tag{4.35}$$

where $h > 1$.

Based on (4.35), Alon and Milman (1985) also derive a second bound

$$b \leq (1 - a)\exp\left(-\ln(1 + 2a)\left[h\sqrt{\frac{\mu_{N-1}}{2d_{\max}}}\right]\right) \tag{4.36}$$

where $[x]$ denotes the largest integer smaller than or equal to x.

Proof: The idea is to construct subsets A_r of $\mathcal{N}$ that include, beside the original subset A, additional nodes of $\mathcal{N}$ within distance $r \in \mathbb{R}$ hops from A, i.e., $A_r = \{v \in \mathcal{N} : d(v, A) \leq r\}$. We construct a sequence on distance $r = j\beta$ for $j = 0, 1, \ldots, k$ of those subsets such that $A_{j\beta}$ and $\mathcal{N}\backslash A_{(j+1)\beta}$ are more than $h > 1$ hops separated, which requires that $h > \beta > 1$. For those subsets $A \subset A_\beta \subset A_{2\beta} \subset \cdots A_{k\beta} \subseteq \mathcal{N}$, application of (4.35) yields

$$1 - a_{(j+1)\beta} = \frac{1 - a_{j\beta}}{1 + \frac{a_{j\beta}h^2\mu_{N-1}}{d_{\max}}} \leq \frac{1 - a_{j\beta}}{1 + a\frac{\beta^2\mu_{N-1}}{d_{\max}}}$$

The largest possible k is such that $k\beta \leq \rho$, where ρ is the diameter of the graph. Now, with (4.20), we observe that, for $N \geq 2$,

$$\frac{1}{\mu_{N-1}} \geq \frac{N-1}{N}\frac{1}{d_{\min}} \geq \frac{1}{2d_{\max}}$$

such that $\frac{2d_{\max}}{\mu_{N-1}} > 1$. Let $\beta^2 = \frac{2d_{\max}}{\mu_{N-1}} > 1$, then

$$1 - a_{(j+1)\beta} \leq (1 - a_{j\beta})\frac{1}{1 + 2a}$$

for $0 \le j < k$. Multiplying those inequalities yields

$$1 - a_{k\beta} \le (1-a)\frac{1}{(1+2a)^k} = (1-a)e^{-k\ln(1+2a)}$$

and by construction $B \subseteq \mathcal{N}\backslash A_{k\beta}$ or $b < 1 - a_{k\beta}$ and $k < \frac{\rho}{\beta} = \rho\sqrt{\frac{\mu_{N-1}}{2d_{\max}}}$. This proves (4.36) for any $h < \rho$. $\square$

101. *Isoperimetric constant η.* If we choose the set B equal to $\mathcal{N}\backslash\mathcal{N}_A$, then $\mathcal{L} - \mathcal{L}_A - \mathcal{L}_B$ is the set of links with one end in A and the other in B. Thus, $\partial A = L - L_A - L_B$ is the number of links between A and its complement $\mathcal{N}\backslash\mathcal{N}_A$. The isoperimetric constant of the graph G is defined[5] as

$$\eta = \min_{\mathcal{N}_A} \frac{\partial A}{N_A} \tag{4.37}$$

where the minimum is over all non empty subsets $\mathcal{N}_A$ of $\mathcal{N}$ satisfying $N_A \le \left[\frac{N}{2}\right]$. The isoperimetric constant is also called the *Cheeger constant*.

The Alon Milman bound (4.33) reduces (with $h = 1$) to

$$\mu_{N-1} \le \partial A\left(\frac{1}{N_A} + \frac{1}{N - N_A}\right)$$

If we denote $\eta_k = \min_{\mathcal{N}_A}\left\{\frac{\partial A}{N_A} \middle| N_A = k\right\}$, then $\mu_{N-1} \le \frac{\partial A}{k}\frac{N}{N-k}$ and this inequality holds for any set N_A, also for the minimizer of the right hand side. Thus, $\mu_{N-1} \le \eta_k \frac{N}{N-k}$ and

$$\frac{N-k}{N}\mu_{N-1} \le \eta_k$$

We may further minimize both sides over all $k = 1, 2, \ldots, \left[\frac{N}{2}\right]$. Observe that $\eta = \min_{1 \le k \le \left[\frac{N}{2}\right]} \eta_k$. Hence, the Alon Milman bound (4.33) leads to a lower bound for the isoperimetric constant

$$\frac{\mu_{N-1}}{2} \le \eta$$

Using Alon's machinery of **art.** 94 that led to the lower bound (4.28), Mohar (1989) showed that, for $N > 3$,

$$\eta \le \sqrt{\mu_{N-1}(2d_{\max} - \mu_{N-1})}$$

102. *Expanders.* A graph G with N nodes is a c expander if every subset $\mathcal{N}_A$ with $N_A \le \left[\frac{N}{2}\right]$ nodes is connected to its complement $\mathcal{N}\backslash\mathcal{N}_A$ by at least cN_A links. Since $\partial A \ge cN_A$, **art.** 101 indicates that $c = \eta$. Expanders are thus very difficult to disconnect because every set of nodes in G is well connected to its complement. This "robustness" property makes expanders highly desirable in the design of fault tolerant networks such as man made infrastructures like communications networks

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[5] The computation of the isoperimetric constant is an NP-complete problem as shown by Mohar (1989).

and electric power transmission networks. A part of the network can only be cut off by destroying a large number of individual connections. In particular, sparse expanders, graphs with few links, have great interest, because the cost of a network usually increases with the number of links.

A well studied subclass of expanders are regular graphs. In Govers *et al.* (2008), Wigderson mentions that almost every regular graph with degree $r \geq 3$ is an ex pander. The proof is probabilistic and does not provide insight how to construct a regular c expander. Although nearly any regular graph is an expander, it turns out that there are only few methods to construct them explicitly. It follows from the bounds in **art.** 101 and $c = \eta$ that

$$\frac{1}{2}\mu_{N-1} \leq c \leq \sqrt{\mu_{N-1}(2r - \mu_{N-1})}$$

where $\mu_{N-1} = r - \lambda_2(A)$ also equals the spectral gap (**art.** 55 and **art.** 74). The larger the spectral gap or the smaller $\lambda_2(A)$, the larger c and the stronger or the more robust the expander is. A remarkable achievement is the discovery that, for all r regular graphs, $\lambda_2(A) \geq 2\sqrt{r-1}$ and that equality is only attained in Ramanujan graphs, where $r - 1$ is a prime power, as shown by Lubotzky *et al.* (1988).

103. *Graph partioning.* Since $rI - Q$ is a non negative matrix for $r > d_{\max}$, a direct application of Fiedler's Theorem 40 in **art.** 171 for $k = 2$ shows that a connected graph G can be partitioned into two distinct, connected components G_1 and G_2, where the nodes of $G_1 = G \backslash G_2$ are elements of the set $\mathcal{M} = \left\{ j \in \mathcal{N} : (x_{N-1})_j \geq \alpha \right\}$, where x_{N-1} is the eigenvector belonging to the second smallest eigenvalue μ_{N-1} of the Laplacian Q and α is some threshold value that specifies different disjoint partitions. Clearly, if $\alpha > \max_{1 \leq j \leq N} (x_{N-1})_j$ or if $\alpha < \min_{1 \leq j \leq N} (x_{N-1})_j$, there is only the "trivial" partition consisting of the original graph G itself. Fiedler (1975) demonstrates that, by varying the threshold $\alpha \geq 0$, all possible cuts that separate the graph $G = G_1 \cup G_2$ into two distinct ($G_1 \cap G_2 = \varnothing$) connected components G_1 and G_2 can be obtained in this way.

Art. 67 indicates that the sum over all positive vector components equals the sum over all negative ones. This means that the value $\alpha = 0$ in Fiedler's partitioning algorithm divides the graph into two "equivalent" partitions, where "equivalent" is measured with respect to the second smallest Laplacian eigenvector. It does not imply, however, that both partitions have the same number of nodes.

4.4 The modularity and the modularity matrix M

104. *Modularity.* The modularity, proposed by Newman and Girvan (2004), is a measure of the quality of a particular division of the network. The modularity is proportional to the number of links falling within clusters or groups minus the expected number in an equivalent network with links placed at random. Thus, if the number of links within a group is no better than random, the modularity is zero.

A modularity approaching one reflects networks with strong community structure: a dense intra group and a sparse inter group connection pattern.

If links are placed at random, then the expected number of links between node i and node j equals $\frac{d_i d_j}{2L}$. The modularity m is defined by Newman (2006) as

$$m = \frac{1}{2L} \sum_{i=1}^{N} \sum_{j=1}^{N} \left(a_{ij} - \frac{d_i d_j}{2L} \right) 1_{\{i \text{ and } j \text{ belong to the same cluster}\}} \tag{4.38}$$

We consider first a network partitioning into two clusters or subgraphs as in **art. 96**. The condition (indicator function) is rewritten in terms of the y vector, defined in **art. 96**, as

$$1_{\{i \text{ and } j \text{ belong to the same cluster}\}} = \frac{1}{2} (y_i y_j + 1)$$

so that

$$m = \frac{1}{4L} \sum_{i=1}^{N} \sum_{j=1}^{N} \left(a_{ij} - \frac{d_i d_j}{2L} \right) y_i y_j$$

because, by the basic law for the degree (2.3) and by (2.2),

$$\sum_{j=1}^{N} \left(a_{ij} - \frac{d_i d_j}{2L} \right) = \sum_{j=1}^{N} a_{ij} - \frac{d_i}{2L} \sum_{j=1}^{N} d_j = 0 \tag{4.39}$$

Clearly, if there is only one partition to which all nodes belong, then $y = u$ and the modularity is $m = 0$ as follows from (4.39).

After defining the symmetric modularity matrix M with elements $m_{ij} = a_{ij} - \frac{d_i d_j}{2L}$, such that

$$M = A - \frac{1}{2L} d.d^T \tag{4.40}$$

we rewrite the modularity m, with respect to a partitioning into two clusters spec ified by the vector y, as a quadratic form

$$m = \frac{1}{4L} y^T M y$$

which is analogous to the number of links R in (4.30) between the two disjoint partitions.

Generally, for a partitioning of the network into c clusters, instead of the vector y, the $N \times c$ community matrix S, defined in **art. 14**, can be used to rephrase the condition as

$$1_{\{i \text{ and } j \text{ belong to the same cluster}\}} = \sum_{k=1}^{c} S_{ik} S_{jk}$$

which leads to the matrix representation of the modularity

$$m = \frac{1}{2L} \sum_{k=1}^{c} \sum_{i=1}^{N} \sum_{j=1}^{N} S_{ik} m_{ij} S_{jk} = \frac{\text{trace} \left(S^T M S \right)}{2L} \tag{4.41}$$

We define the community vector s_k as the k th column of the community matrix S, which specifies the k th cluster: all components of s_k, corresponding to nodes belonging to cluster C_k, are equal to one, otherwise they are zero. For $c = 2$ clusters, we note that the vector $y = s_1 - s_2$, and that, in case $c = 2$, only one vector suffices for the partitioning, instead of s_1 and s_2.

Using the eigenvalue decomposition (**art.** 156) of the symmetric modularity matrix $M = W \text{diag}(\lambda_j(M)) W^T$, where W is the orthogonal $N \times N$ matrix with the j th eigenvector w_j belonging to $\lambda_j(M)$ in column j, the general spectral expression for the modularity m for any number of clusters c follows from (4.41) as

$$m = \frac{\text{trace}\left((W^T S)^T \text{diag}(\lambda_j(M)) W^T S\right)}{2L}$$
$$= \frac{1}{2L} \sum_{j=1}^{N} \left(\sum_{k=1}^{c} (w_j^T s_k)^2 \right) \lambda_j(M) \tag{4.42}$$

because $(W^T S)_{jk} = \sum_{q=1}^{N} W_{qj} S_{qk} = w_j^T s_k$. In particular, the scalar product $w_j^T s_k = \sum_{q \in C_k} (w_j)_q$ is the sum of those eigenvector components of w_j that belong to cluster C_k. If we write the community vector as a linear combination of the eigenvectors of M, $s_k = \sum_{j=1}^{N} \beta_{kj} w_j$, then the orthogonality of eigenvectors indicates that the coefficients equal $\beta_{kj} = w_j^T s_k$. Moreover, **art.** 14 shows that the vectors $s_1, s_2, \ldots, s_c$ are orthogonal vectors, and, by definition, that $\sum_{k=1}^{c} s_k = u$. Since u is an eigenvector of M belonging to the zero eigenvalue as follows from (4.39), we observe that

$$\sum_{k=1}^{c} w_j^T s_k = 0$$

provided the eigenvector $w_j \neq u$. Using the Cauchy identity (8.86)

$$c \sum_{k=1}^{c} (w_j^T s_k)^2 - \left(\sum_{k=1}^{c} w_j^T s_k \right)^2 = \sum_{m=2}^{c} \sum_{k=1}^{m-1} (w_j^T (s_m - s_k))^2$$

we find that

$$m = \frac{1}{2Lc} \sum_{j=1}^{N} \left(\sum_{m=2}^{c} \sum_{k=1}^{m-1} (w_j^T (s_m - s_k))^2 \right) \lambda_j(M)$$

which reduces for $c = 2$ and $y = s_1 - s_2$ to (4.60) below.

Since $WW^T = I$ (**art.** 151), we have that $\text{trace}\left((W^T S)^T W^T S\right) = \text{trace}(S^T S) = N$ (**art.** 14), such that we obtain a companion of (4.42)

$$\sum_{j=1}^{N} \sum_{k=1}^{c} (w_j^T s_k)^2 = N \tag{4.43}$$

Let $w_q = \frac{u}{\sqrt{N}}$ denote the eigenvector of M belonging to the eigenvalue $\lambda_q(M) = 0$,

then

$$\sum_{k=1}^{c} \left(w_q^T s_k\right)^2 = \frac{1}{N} \sum_{k=1}^{c} \left(u^T s_k\right)^2 = \frac{1}{N} \sum_{k=1}^{c} n_k^2$$

where n_k is the number of nodes in cluster C_k. Invoking the inequality (3.39) to (4.42) subject to (4.43) yields

$$\frac{\sum_{j=1;j\neq q}^{N} \left(\sum_{k=1}^{c} \left(w_j^T s_k\right)^2\right) \lambda_j (M)}{\sum_{j=1;j\neq q}^{N} \sum_{k=1}^{c} \left(w_j^T s_k\right)^2} \leq \max_{1 \leq j \leq N} \frac{\left(\sum_{k=1}^{c} \left(w_j^T s_k\right)^2\right) \lambda_j (M)}{\sum_{k=1}^{c} \left(w_j^T s_k\right)^2} = \lambda_1 (M)$$

from which we find, with $E[D] = \frac{2L}{N}$, a spectral upper bound for the modularity

$$m \leq \frac{\lambda_1 (M)}{E[D]} \left(1 - \frac{1}{N^2} \sum_{k=1}^{c} n_k^2\right) \tag{4.44}$$

This bound can also be written as

$$m \leq \frac{\lambda_1 (M)}{E[D]} \left(1 - \frac{1}{c} - \frac{c}{N^2} \mathrm{Var}[n_C]\right)$$

where n_C is the number of nodes in an arbitrary cluster, because $E[n_C] = \frac{1}{c} \sum_{k=1}^{c} n_k = \frac{N}{c}$.

105. *Upper bound for the modularity.* The general definition (4.38) is first rewritten as follows. We transform the nodal representation to a counting over links $l = i \sim j$ such that

$$\sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} 1_{\{i \text{ and } j \text{ belong to the same cluster}\}} = 2 \sum_{k=1}^{c} L_k$$

where L_k is the number of links of cluster C_k, and the factor 2 arises from the fact that all links are counted twice, due the symmetry $A = A^T$ of the adjacency matrix. If we denote by L_{inter} the number of inter community links, i.e. the number of links that are cut by partitioning the network into c communities or clusters, then

$$L = \sum_{k=1}^{c} L_k + L_{\text{inter}}$$

Similarly,

$$\sum_{i=1}^{N} \sum_{j=1}^{N} d_i d_j 1_{\{i \text{ and } j \text{ belong to the same cluster}\}} = \sum_{k=1}^{c} \left(\sum_{i \in C_k} d_i\right) \left(\sum_{j \in C_k} d_j\right) = \sum_{k=1}^{c} D_{C_k}^2$$

where

$$D_{C_k} = \sum_{i \in C_k} d_i$$

is the sum of the degrees of all nodes that belong to cluster C_k. Clearly, $D_{C_k} \geq 2L_k$, because some nodes in cluster C_k may possess links connected to nodes in

other clusters. The basic law of the degree (2.3) then shows that $\sum_{k=1}^{c} D_{C_k} = 2L$. Substituting these expressions in the definition (4.38) leads to an alternative expression[6] for the modularity

$$m = \sum_{k=1}^{c} \left(\frac{L_k}{L} - \left(\frac{D_{C_k}}{2L} \right)^2 \right) \tag{4.45}$$

Subject to the basic law of the degree, $\sum_{k=1}^{c} D_{C_k} = 2L$, the sum $\sum_{k=1}^{c} D_{C_k}^2$ is maximized when $D_{C_k} = \frac{2L}{c}$ for all $1 \le k \le c$. Indeed, the corresponding Lagrangian

$$\mathcal{L} = \sum_{k=1}^{c} D_{C_k}^2 + \xi \left(\sum_{k=1}^{c} D_{C_k} - 2L \right)$$

where ξ is a Lagrange multiplier, supplies the set of equations for the optimal solution, $\frac{\partial \mathcal{L}}{\partial D_{C_j}} = 2D_{C_j} + \xi = 0$ for $1 \le j \le c$ and $\frac{\partial \mathcal{L}}{\partial \xi} = \sum_{k=1}^{c} D_{C_k} - 2L = 0$, which is satified for $\xi = -\frac{4L}{c}$ and $D_{C_j} = \frac{2L}{c}$ for all $1 \le j \le c$. Hence, $\sum_{k=1}^{c} D_{C_k}^2 \le \frac{(2L)^2}{c}$. The modularity in (4.45) is minimized, for $c > 1$, if $L_k = 0$ for $1 \le k \le c$ and $\sum_{k=1}^{c} D_{C_k}^2$ is maximized such that $m \ge -\frac{1}{c}$. In conclusion, the modularity of any graph is never smaller than $-\frac{1}{2}$, and this minimum is obtained for the complete bipartite graph.

Invoking the Cauchy identity (8.86) and $\sum_{k=1}^{c} D_{C_k} = 2L$,

$$\sum_{k=1}^{c} D_{C_k}^2 = \frac{(2L)^2}{c} + \frac{1}{c} \sum_{j=2}^{c} \sum_{k=1}^{j-1} \left(D_{C_j} - D_{C_k} \right)^2$$

results in yet another expression for the modularity

$$m = 1 - \frac{L_{\text{inter}}}{L} - \frac{1}{c} - \frac{1}{c} \sum_{j=2}^{c} \sum_{k=1}^{j-1} \left(\frac{D_{C_j} - D_{C_k}}{2L} \right)^2 \tag{4.46}$$

Since the double sum is always positive, (4.46) provides us with an upper bound for the modularity,

$$m \le 1 - \frac{1}{c} - \frac{L_{\text{inter}}}{L} \tag{4.47}$$

The upper bound (4.47) is only attained if the degree sum of all clusters is the same. In addition, the upper bound (4.47) shows that $m \le 1$ and that a modularity of 1 is only reached asymptotically, when the number of clusters $c \to \infty$ and $L_{\text{inter}} = o(L)$, implying that the fraction of inter community links over the total number of links L is vanishingly small for large graphs ($N \to \infty$ and $L \to \infty$).

Let $D_{\Delta C} = \max_{\{C_j, C_k\}} |D_{C_j} - D_{C_k}|$, then a lower bound of the modularity, deduced from (4.46), is

$$m \ge 1 - \frac{L_{\text{inter}}}{L} - \frac{1}{c} - \frac{(c-1)}{2} \left(\frac{D_{\Delta C}}{2L} \right)^2 \tag{4.48}$$

---

[6] Newman (2010) presents still another expression for the modularity.

Only if $D_{\Delta C} = 0$, the lower bound (4.48) equals the upper bound (4.47) and the equality sign can occur. Excluding the case that $D_{\Delta C} = 0$, then not all D_{C_j} are equal, and we may assume an ordering $D_{C_1} \geq D_{C_2} \geq \ldots \geq D_{C_c}$, with at least one strict inequality. We demonstrate that, for $c > 2$, not all differences $D_{C_j} - D_{C_k} = D_{\Delta C} > 0$ for any pair (j, k). For, assume the contrary so that $D_{C_1} - D_{C_2} = D_{C_2} - D_{C_3} = D_{C_1} - D_{C_3} = D_{\Delta C} > 0$, then $D_{\Delta C} = D_{C_1} - D_{C_3} = (D_{C_1} - D_{C_2}) + (D_{C_2} - D_{C_3}) = 2D_{\Delta C}$, which cannot hold for $D_{\Delta C} > 0$. Hence, if $D_{\Delta C} > 0$, the inequality in (4.48) is strict; alternatively, the lower bound (4.48) is not attainable in that case.

In order for a network to have modular structure, the modularity must be positive. The requirement that the lower bound (4.48) is non negative, supplies us with an upper bound for the maximum difference $D_{\Delta C}$ in the nodal degree sum between two clusters in a "modular" graph

$$D_{\Delta C} \leq 2L \sqrt{\frac{2}{c-1} \left(1 - \frac{L_{\text{inter}}}{L} - \frac{1}{c}\right)} \tag{4.49}$$

For $c > 1$, (4.49) demonstrates that $D_{\Delta C} < 2L$. Ignoring the integer nature of c, the lower bound (4.48) is maximized with respect to the number of clusters c when

$$c^* = \frac{2\sqrt{2}L}{D_{\Delta C}} > \sqrt{2} \tag{4.50}$$

resulting in

$$m \geq 1 - \frac{L_{\text{inter}}}{L} - \sqrt{2}\left(\frac{D_{\Delta C}}{2L}\right) + \frac{1}{2}\left(\frac{D_{\Delta C}}{2L}\right)^2$$

The right hand side in this lower bound is positive provided that $1 > \frac{D_{\Delta C}}{2L} > \sqrt{2}\left(1 - \sqrt{\frac{L_{\text{inter}}}{L}}\right)$. When this lower bound for $\frac{D_{\Delta C}}{2L}$ is satisfied, the modularity m is certainly positive, implying that the graph exhibits modular structure.

106. *Spectrum of the modularity matrix M.* Since the row sum (4.39) of the modularity matrix M is zero, which translates to $Mu = 0$, the modularity matrix has a zero eigenvalue corresponding to the eigenvector u, similar to the Laplacian matrix (**art. 2**). Unlike the Laplacian Q, the modularity matrix M always has negative eigenvalues. Indeed, from (8.7) and **art. 25**, the sum of the eigenvalues of M equals

$$\sum_{j=1}^{N} \lambda_j (M) = -\frac{1}{2L} \sum_{j=1}^{N} d_j^2 = -\frac{N_2}{N_1} \tag{4.51}$$

where N_k is the total number of walks of length k (**art. 33**). With a little more effort, we find that

$$\sum_{j=1}^{N} \lambda_j^2 (M) = \text{trace}\left(A^2\right) - \frac{1}{L}\text{trace}\left(Add^T\right) + \frac{1}{(2L)^2} \sum_{j=1}^{N} d_j^2 \text{trace}\left(d.d^T\right)$$

Using (3.5) and **art. 33**, we have

$$\sum_{j=1}^{N} \lambda_j^2(M) = 2L - \frac{1}{L} d^T A d + \left(\frac{1}{2L}\sum_{j=1}^{N} d_j^2\right)^2 = N_1 - \frac{2N_3}{N_1} + \left(\frac{N_2}{N_1}\right)^2 \qquad (4.52)$$

In general, M and A do not commute, similar to the fact that Q and A also do not commute. Hence, **art. 184** shows that the set of eigenvectors $\{w_k\}_{1 \le k \le N}$ of M is different from the set of eigenvectors $\{x_k\}_{1 \le k \le N}$ of A.

The eigenvalues of the modularity matrix $M = A - \frac{1}{2L} d.d^T$ are zeros of the characteristic polynomial

$$\det(M - \lambda I) = \det\left(A - \lambda I - \frac{1}{2L} d.d^T\right)$$
$$= \det(A - \lambda I)\det\left(I - \frac{1}{2L}(A - \lambda I)^{-1} d.d^T\right)$$

Using the "rank one update" formula (8.82), we have

$$\det(M - \lambda I) = \det(A - \lambda I)\left(1 - \frac{1}{2L} d^T (A - \lambda I)^{-1} d\right) \qquad (4.53)$$

We invoke the resolvent (8.66) in **art. 178**

$$d^T(A - \lambda I)^{-1} d = \sum_{m=1}^{N} \frac{(d^T x_m)^2}{\lambda_m - \lambda}$$

where x_m is the eigenvector of A belonging to eigenvalue λ_m. Since $d^T x_m = u^T A x_m = \lambda_m u^T x_m$, we obtain

$$1 - \frac{1}{2L} d^T(A - \lambda I)^{-1} d = \frac{1}{2L}\left\{2L - \sum_{m=1}^{N} \frac{\lambda_m^2 (u^T x_m)^2}{\lambda_m - \lambda}\right\}$$

Using $N_1 = 2L$ and (3.11),

$$1 - \frac{1}{2L} d^T(A - \lambda I)^{-1} d = \frac{1}{2L}\left\{\sum_{m=1}^{N} \lambda_m (u^T x_m)^2 - \sum_{m=1}^{N} \frac{\lambda_m^2 (u^T x_m)^2}{\lambda_m - \lambda}\right\}$$
$$= \frac{-\lambda}{2L}\sum_{m=1}^{N} \frac{(u^T x_m)^2 \lambda_m}{\lambda_m - \lambda}$$

which can, in view of (3.17), be written in terms of the generating function $N_G(z)$ of the total number of walks (**art. 34**). Thus, we arrive at[7]

$$\det(M - \lambda I) = \frac{\lambda}{2L}\det(A - \lambda I)\left(N_G\left(\frac{1}{\lambda}\right) - N\right) \qquad (4.54)$$

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[7] Invoking (3.20) and $c_A(\lambda)$ $\det(A - \lambda I)$, another expression for the characteristic polynomial is

$$\det(M - \lambda I) \quad \frac{\lambda}{2L}\left((-1)^N \lambda c_{A^c}(-\lambda - 1) - (\lambda + N) c_A(\lambda)\right)$$

Since $\lim_{\lambda \to 0} N_G \left(\frac{1}{\lambda} \right) = 0$, the characteristic polynomial (4.54) of M illustrates that $\lambda = 0$ is an eigenvalue of M, corresponding to the eigenvalue u as shown above. By a same argument as in **art. 180**, the function $g(\lambda) = 1 - \frac{1}{2L} d^T (A - \lambda I)^{-1} d = N_G \left(\frac{1}{\lambda} \right) - N$ has simple zeros that lie in between two consecutive eigenvalues of the adjacency matrix A.

In summary, the eigenvalues of the modularity matrix M interlace with the eigenvalues of adjacency matrix A: $\lambda_1 (A) \geq \lambda_1 (M) \geq \lambda_2 (A) \geq \lambda_2 (M) \geq \dots \geq \lambda_N (A) \geq \lambda_N (M)$.

107. *Spectrum of the modularity matrix M for regular graphs.* For regular graphs, where each node has degree r and $Au = ru$ (**art. 41**), we have that $(A - \lambda I) u = (r - \lambda) u$ from which $(A - \lambda I)^{-1} u = (r - \lambda)^{-1} u$. Substituted in (4.53) yields, with the degree vector $d = r.u$,

$$\det (M - \lambda I) = \det (A - \lambda I) \left(1 - \frac{r}{N} u^T (A - \lambda I)^{-1} u \right)$$

$$= \det (A - \lambda I) \left(1 - \frac{r}{N (r - \lambda)} u^T u \right) = \frac{\lambda}{\lambda - r} \det (A - \lambda I)$$

After invoking the basic relation (8.5), we arrive at

$$\det (M - \lambda I) = \frac{\lambda}{\lambda - r} \prod_{k=1}^{N} (\lambda_k (A) - \lambda)$$

$$= -\lambda \prod_{k=2}^{N} (\lambda_k (A) - \lambda)$$

Hence, the eigenvalues of the modularity matrix M of a regular graph are precisely equal to the eigenvalues of the corresponding adjacency matrix A, except that the largest eigenvalue $\lambda_1 (A) = r$ is replaced by the eigenvalue at zero.

108. *The largest eigenvalue of the modularity matrix.* Since $N_G \left(\frac{1}{\lambda} \right) - N > 0$ in (4.54) for $\lambda \geq \lambda_1$ as follows from (3.15) in **art. 34**, $\lambda_1 (M) \leq \lambda_1 (A)$. This inequality is also found from the interlacing property of M and A derived in **art. 106**. We will show here that $\lambda_1 (M) < \lambda_1 (A)$.

Since $\lambda = 0$ is always an eigenvalue of M (**art. 106**), there cannot be a smaller largest eigenvalue than zero. The interlacing property bounds the largest eigenvalue from below, $\lambda_1 (M) \geq \lambda_2 (A)$, and **art. 58** demonstrates that all graphs have a non negative second largest eigenvalue $\lambda_2 (A) \geq 0$, except for the complete graph. The modularity matrix of the complete graph K_N is $M_{K_N} = \frac{1}{N} J - I$, whose characteristic polynomial is $\det (M - \lambda I) = (-1)^N \lambda (1 + \lambda)^{N-1}$ as follows from (5.1). This illustrates that the largest eigenvalue of the complete graph is $\lambda_1 (M_{K_N}) = 0$, which is also the smallest possible largest modularity eigenvalue of all graphs.

The eigenvector w_1 of M belonging to $\lambda_1 (M)$ has negative components (in contrast to the largest eigenvector x_1 of A), because $u^T w_1 = 0$, which is similar to the eigenvectors of the Laplacian Q (**art. 67**). The Rayleigh equation (8.28) and the

Rayleigh inequalities in **art.** 152 demonstrate that

$$\lambda_1(M) = \frac{w_1^T M w_1}{w_1^T w_1} = \frac{w_1^T A w_1}{w_1^T w_1} - \frac{1}{2L}\frac{\left(w_1^T d\right)^2}{w_1^T w_1} \le \lambda_1(A) - \frac{1}{2L}\left(w_1^T d\right)^2 \qquad (4.55)$$

because $w_1^T w_1 = 1$ as the orthogonal eigenvectors are normalized (**art.** 151). The scalar product $w_1^T d$ is only zero for regular graphs, where each node has degree r, because the degree vector is $d = r.u$ and $w_1^T u = 0$, provided $w_1 \ne \frac{u}{\sqrt{N}}$ (as in the complete graph). However, **art.** 107 shows that the largest eigenvalue for regular graphs equals $\lambda_1(M_r) = \max(0, \lambda_2(A_r)) < \lambda_1(A_r)$, where the subscript r explicitly refers to regular graphs. Due to interlacing (**art.** 106), of all graphs, the regular graph has the smallest largest eigenvalue of the modularity matrix. Because the last term in the above upper bound is always strictly positive for non regular graphs, we obtain the range of $\lambda_1(M)$ for any graph: $0 \le \lambda_1(M) < \lambda_1(A)$. In summary, the largest eigenvalue of the modularity matrix M is always strictly smaller than the largest eigenvalue of the corresponding adjacency matrix A.

For non regular graphs, the degree vector d is not proportional to the eigenvector u of M (**art.** 41) and $w_1^T d \ne 0$. We can write the degree vector d as a linear combination of the eigenvectors of M,

$$d = \sum_{k=1}^N \gamma_k w_k \qquad \text{where } \gamma_k = d^T w_k \qquad (4.56)$$

Let $w_q = \frac{u}{\sqrt{N}}$, then $d^T u = 2L = \sqrt{N}\gamma_q$ and $\gamma_q > \gamma_k$ for $1 \le k \ne q \le N$ by a similar argument as in **art.** 38. In addition, we have $d^T d = \sum_{k=1}^N \gamma_k^2$ and $d^T d - N\left(\frac{2L}{N}\right)^2 = N\mathrm{Var}[D] > 0$, such that

$$\frac{1}{2L}\left(w_1^T d\right)^2 = \frac{\mathrm{Var}[D]}{E[D]} - \frac{1}{2L}\sum_{k=2;k\ne q}^N \gamma_k^2$$

Unfortunately, it is difficult to estimate the last sum in order to provide a good lower bound for $\gamma_1^2 = \left(w_1^T d\right)^2$ in (4.55).

Next, we apply the Rayleigh principle to the adjacency matrix A,

$$\lambda_1(A) = \frac{x_1^T A x_1}{x_1^T x_1} = \frac{x_1^T M x_1}{x_1^T x_1} + \frac{1}{2L}\left(x_1^T d\right)^2 \le \lambda_1(M) + \frac{1}{2L}\left(x_1^T d\right)^2 \qquad (4.57)$$

Combining both Rayleigh inequalites (4.57) and (4.55), we obtain bounds for the difference $\lambda_1(A) - \lambda_1(M) > 0$,

$$\frac{1}{2L}\left(w_1^T d\right)^2 \le \lambda_1(A) - \lambda_1(M) \le \frac{1}{2L}\left(x_1^T d\right)^2$$

Since $x_1^T d = x_1^T A^T u = (A x_1)^T u = \lambda_1(A) x_1^T u$, we arrive from (4.57) at the lower bound

$$\lambda_1(A)\left\{1 - \frac{\left(x_1^T u\right)^2}{2L}\lambda_1(A)\right\} \le \lambda_1(M)$$

which is only useful when the term in brackets is positive, $\left(x_1^T u\right)^2$ can be determined accurately[8] and when the lower bound is larger than $\lambda_2(A)$. On the other hand, the scalar product $x_1^T d$ is maximal if $x_1 = \frac{d}{\sqrt{d^T d}}$, such that, using (4.51),

$$\frac{1}{2L}\left(x_1^T d\right)^2 \le \frac{d^T d}{2L} = \frac{N_2}{N_1} = -\sum_{j=1}^{N} \lambda_j(M)$$

from which we obtain, together with (4.57), the upper bound

$$\lambda_1(A) \le -\sum_{j=2}^{N} \lambda_j(M)$$

109. *Bounds for the largest eigenvalue of the modularity matrix.* Since $d^T M d = d^T A d - \frac{1}{2L}\left(d^T d\right)^2 = N_3 - \frac{N_2^2}{N_1}$, we obtain with (4.56)

$$N_3 - \frac{N_2^2}{N_1} = \sum_{k=1}^{N} \gamma_k^2 \lambda_k(M) \tag{4.58}$$

As shown in Section 7.5, the sign of (4.58) determines whether a graph is assortative (positive sign) or disassortative (negative sign). Similarly, from $d^T M^2 d$, we deduce that

$$N_4 - 2\frac{N_3 N_2}{N_1} + \frac{N_2^3}{N_1^2} = \sum_{k=1}^{N} \gamma_k^2 \lambda_k^2(M)$$

By applying the inequality (3.39), we obtain

$$\frac{N_3}{N_2} - \frac{N_2}{N_1} = \frac{\sum_{k=1}^{N} \gamma_k^2 \lambda_k(M)}{\sum_{k=1}^{N} \gamma_k^2} \le \max_{1 \le k \le n} \frac{\gamma_k^2 \lambda_k(M)}{\gamma_k^2} = \lambda_1(M)$$

and

$$\frac{N_4}{N_2} - 2\frac{N_3}{N_1} + \left(\frac{N_2}{N_1}\right)^2 \le \lambda_1^2(M)$$

Application of Laguerre's Theorem 64, combined with **art.** 198 and trace relations (4.51) and (4.52), yields the rather complicated upper bound

$$\lambda_1(M) \le -\frac{1}{N}\left(\frac{N_2}{N_1}\right) + \frac{N-1}{N}\sqrt{\left(\frac{N_2}{N_1}\right)^2 - \frac{N}{N-1}\left(\frac{2N_3}{N_1} - N_1\right)} \tag{4.59}$$

For regular graphs where $N_k = Nr^k$ and $0 < \lambda_1(M_r) = \lambda_2(A_r)$, the bound (4.59) provides an upper bound for the second largest eigenvalue of the adjacency matrix,

$$\lambda_2(A_r) \le -\frac{r}{N} + \frac{1}{N}\sqrt{r(N-1)}\sqrt{N^2 - (N+1)r}$$

---

[8] Indeed, the bound $\left(x_1^T u\right)^2 \le N$, as shown in **art.** 38, leads to a lower bound $\lambda_1(A)$ $\frac{\lambda_1^2(A)}{E[D]} \le \lambda_1(M)$, that is smaller than zero for non-regular graphs and, thus, useless.

For the complete graph K_N, where $r = N - 1$ and $\lambda_1(M_{K_N}) = 0$, the bound (4.59) is exact. In view of the upper bound (4.44) for the modularity, the bound (4.59) is only useful when the right hand side is smaller than the average degree $E[D]$. Numerical evaluations indicate that the bound (4.59) is seldom sharp.

110. *Maximizing the modularity.* Maximizing the modularity m consists of finding the best $N \times c$ community matrix S in either definition (4.41) or (4.42). Numerous algorithms, that (approximately for $c > 2$) find the best community matrix S, exist, for which we refer to Newman (2010). Here, we concentrate on a spectral method.

Starting from the quadratic form $m = \frac{1}{4L} y^T M y$ for the modularity, where the number of clusters $c = 2$, Newman (2006) mimics the method in **art.** 96 by writing the vector $y = \sum_{j=1}^{N} \beta_j w_j$ with $\beta_j = y^T w_j$ as a linear combination of the orthogonal eigenvectors $w_1, w_2, \ldots, w_N$ of M,

$$m = \frac{1}{4L} \sum_{j=1}^{N} \beta_j^2 \lambda_j(M) \tag{4.60}$$

Maximizing the modularity m is thus equal to choosing the vector y as a linear combination of the few largest eigenvectors, such that components of y are either -1 and $+1$, which is difficult as mentioned above in **art.** 96. Newman (2006) proposes to maximize $\beta_1 = y^T w_1$ and the maximum $\beta_1 = \sum_{j=1}^{N} \left|(w_1)_j\right|$ is reached when each component $y_j = -1$ if $(w_1)_j < 0$ or $y_j = 1$ if $(w_1)_j \geq 0$. Moreover, using properties of norms (**art.** 162), we find that $\beta_1 = \|w_1\|_1 \geq \|w_1\|_2 = 1$, and by construction and the orthogonality of the eigenvectors, $\beta_j < \|w_j\|_1$.

This separation of nodes into two partitions according to the sign of the vector components in the largest eigenvector w_1 of M is similar in spirit to Fiedler's algorithm (**art.** 103). Apart from the sign considered so far, a large eigenvector component contributes more to the modularity m in (4.60) than a small (in absolute value) component. Thus, the magnitude (in absolute value) of the components in w_1 measure how firmly the corresponding node in the graph belongs to its assigned group, which is a general characteristic of a class of spectral measures called "eigenvalue centralities", defined in Section 7.8.1.

Notice that, since u is the eigenvector belonging to $\lambda(M) = 0$, the trivial partition of whole the network in one group, is excluded from modularity (because $\lambda(M) = 0$ does not contribute to the sum in (4.60)) and that any other eigenvector, due to the orthogonality (**art.** 151), must have at least one negative component. In contrast to the Fiedler partitioning based on the Laplacian, the situation where all non zero eigenvalues of M are negative might occur (as in the complete graph, for example; **art.** 108), which indicates that there is no partition, except for the trivial one, and that the modularity m in (4.60) is negative. This observation is important: Newman (2006) exploits the fact that $m < 0$ to *not* partition a (sub)network.

111. *Newman's iterated bisection.* Let us now consider a network partitioning in more than two clusters or groups. Usually, as in Fiedler's approach, we partition

the graph first into two subgraph, then apply Fiedler's algorithm recursively to each subgraph, which is divided again into two parts, and so on. Newman (2006) remarks that deleting the links between the two partitions, and then applying the second iteration of partitioning into two parts, is not correct, because the modularity in (4.38) will change if links are deleted. Instead, Newman proposes to write the additional contribution Δm to the modularity upon further dividing a group g of N_g nodes into two as

$$
\Delta m = \frac{1}{4L} \left(\sum_{i,j \in g} m_{ij} y_i y_j - \sum_{i,j \in g} m_{ij} \right)
$$
$$
= \frac{1}{4L} \sum_{i,j \in g} \left(m_{ij} - \delta_{ij} \sum_{k \in g} m_{ik} \right) y_i y_j = \frac{1}{4L} y_g^T M_g y_g \qquad (4.61)
$$

where the $N_g \times N_g$ symmetric matrix M_g has elements $(M_g)_{ij}$ indexed by the links (i,j) within the group g,

$$
(M_g)_{ij} = m_{ij} - \delta_{ij} \sum_{k \in g} m_{ik}
$$

We note that $M_g u = \sum_{j \in g} m_{ij} - \sum_{j \in g} \delta_{ij} \sum_{k \in g} m_{ik} = 0$ and that $\sum_{k \in g} m_{ik} = 0$ for all i, only if $g = G$, because then $Mu = 0$, implying that this sum vanishes in the first step of partitioning process (as in (4.38)). Hence, M_g formally possesses the same properties as M and we can apply the above spectral algorithm derived from (4.60) to further partition the group g into two parts, provided M_g has positive eigenvalues. Since g is a subgraph of G, the Interlacing Theorem 42 states that the eigenvalues of M_g interlace with those of M, such that subsequent divisions have a smaller impact on the modularity. As explained above, if M_g has non positive eigenvalues, the group g should not be divided, because the contribution Δm to the total modularity should be positive, else nothing is gained. The recursive subpartitioning of a group into two smaller groups is terminated if the eigenvalues of M_g are all non positive, which is an elegant check in Newman's partitioning algorithm. This stopping criterion is sufficient to determine indivisibility of a group, but it is not always necessary. Indeed, when there are a few, small positive and many large negative eigenvalues of M_g, the sum in (4.60) can be negative. We can guard against this possibility by just checking in (4.61) whether $\Delta m \geq 0$. If $\Delta m < 0$, we leave the corresponding subgraph undivided. As a result, the outcome of the algorithm gives subgraphs that are all indivisible, according to the modularity measure.

Finally, we end by mentioning another algorithm that does not involve spectral analysis. Assume some initial split of the graph into two groups. We move a node from one group to the other, only if the resulting modularity increases, and we start preferably with the node whose move has the largest increase in m. We repeatedly move each node once in such way. To be sure that no greater modularity is possible

after one entire round over all the nodes, we can repeat the process iteratively until the modularity cannot further be improved. The best partitioning results according to Newman (2006) seem to be achieved when first the spectral method above is followed up to some broad division of the network, which is then refined by the repeated move algorithm, due to Kerninghan and Lin (1970).

4.5 Bounds for the diameter

112. *Diameter ρ.* Another noteworthy deduction from the Alon Milman bound (4.33) is:

Theorem 15 (Alon-Milman) *The diameter ρ of a connected graph is at most*

$$\rho \leq \left[\sqrt{\frac{2d_{\max}}{\mu_{N\ 1}}} \log_2 N \right] + 1 \tag{4.62}$$

Proof: If B is the set of all nodes of G at a larger distance than h from A and A contains at least half of the nodes ($a \geq \frac{1}{2}$), then (4.36) gives

$$b \leq \frac{1}{2} \exp\left(-\ln(2) \left[h \sqrt{\frac{\mu_{N\ 1}}{2d_{\max}}} \right] \right)$$

If we require that $\exp\left(-\ln(2) \left[h\sqrt{\frac{\mu_{N\ 1}}{2d_{\max}}} \right] \right) \leq \frac{1}{N}$, then $h \leq \sqrt{\frac{2d_{\max}}{\mu_{N\ 1}}} \log_2 N < \left[\sqrt{\frac{2d_{\max}}{\mu_{N\ 1}}} \log_2 N \right] + 1$. By construction, for such h, $b < \frac{1}{N}$ or $B = \varnothing$, which implies that $A = \mathcal{N}$. Next, if $v \in \mathcal{N}$, then the subset $\{v_h\}$ of nodes that is reached within h hops of node v contains more than $N/2$ nodes. Indeed, suppose the converse and define $A = \mathcal{N} \setminus \{v_h\}$. Then $a = A/N > \frac{1}{2}$. But, we have shown that, if $h = \rho$, then $A = \mathcal{N}$. This contradicts the hypothesis. Hence, all nodes in G are reached from an arbitrary node within $h = \rho$ hops, where ρ is specified in (4.62). $\qquad\square$

Theorem 16 (Van Dam-Haemers) *The diameter ρ of a connected graph is at most*

$$\rho \leq \left[\frac{\log 2(N-1)}{\log\left(\sqrt{\mu_1} + \sqrt{\mu_{N\ 1}} \right) - \log\left(\sqrt{\mu_1} - \sqrt{\mu_{N\ 1}} \right)} \right] + 1 \tag{4.63}$$

Proof: The proof is based on the quotient matrix (**art. 15**) of a graph and on interlacing (**art. 182**). $\qquad\square$

Theorem 17 (Mohar) *The diameter ρ of a connected graph is at most*

$$\rho \leq 2 \left[\frac{\log \frac{N}{2}}{\log\left(\frac{d_{\max}+\eta}{d_{\max}\ \eta} \right)} \right] \tag{4.64}$$

where η is the isoperimetric constant.

Proof: Mohar (1989) considers the subsets

$$A_u (r) = \{v \in \mathcal{N} : d(v, u) \le r\}$$

at distance r of node u. The definition (4.37) shows that, for $|A_u (r)| \le \left[\frac{N}{2}\right]$,

$$\eta \left(|A_u (r)| + |A_u (r - 1)|\right) \le \partial A_u (r) + \partial A_u (r - 1)$$

where $\partial A_u (r)$ contains all the links between the set $A_u (r) \backslash A_u (r - 1)$ and the set $A_u (r + 1) \backslash A_u (r)$. Hence, $\partial A_u (r) + \partial A_u (r - 1)$ contains all links in two hop shortest paths between the set $A_u (r - 1) \backslash A_u (r - 2)$ and the set $A_u (r + 1) \backslash A_u (r)$, which equals

$$\partial A_u (r) + \partial A_u (r - 1) = \sum_{v \in A_u(r) \backslash A_u(r\ 1)} d_v \le d_{\max} \left(|A_u (r)| - |A_u (r - 1)|\right)$$

Thus,

$$\eta \left(|A_u (r)| + |A_u (r - 1)|\right) \le d_{\max} \left(|A_u (r)| - |A_u (r - 1)|\right)$$

from which, for $|A_u (r)| \le \left[\frac{N}{2}\right]$,

$$\frac{|A_u (r)|}{|A_u (r - 1)|} \ge \frac{d_{\max} + \eta}{d_{\max} - \eta}$$

Since $|A_u (0)| = 1$ (and $|A_u (1)| = d_u$), iterating yields

$$|A_u (r)| \ge \left(\frac{d_{\max} + \eta}{d_{\max} - \eta}\right)^r$$

provided $|A_u (r)| \le \left[\frac{N}{2}\right]$, which restricts $r_{\max} \le \left\lceil \frac{\log \frac{N}{2}}{\log\left(\frac{d_{\max}+\eta}{d_{\max}\ \eta}\right)} \right\rceil$. This maximum hopcount reaches half of the nodes. To reach also the other half of nodes in the complement, at most $2r_{\max}$ hops are needed, which proves (4.64). $\qquad\square$

4.6 Eigenvalues of graphs and subgraphs

113. If G_1 and G_2 are link disjoint graphs on the same set of nodes, then the union $G = G_1 \cup G_2$ possesses the adjacency matrix $A_G = A_{G_1} + A_{G_2}$ and the Laplacian $Q_G = Q_{G_1} + Q_{G_2}$. **Art.** 183 then states that, for each eigenvalue $1 \le k \le N$,

$$\lambda_N (G_1) + \lambda_k (G_2) \le \lambda_k (G) \le \lambda_k (G_2) + \lambda_1 (G_1)$$
$$\mu_k (G_2) \le \mu_k (G) \le \mu_k (G_2) + \mu_1 (G_1)$$

This shows that the Laplacian eigenvalues $\mu_k (G)$ are non decreasing if links are added in a graph, or, more generally, if $G_2 \subseteq G$ and both have the same number of nodes, $N_{G_2} = N_G$, then $\mu_k (G_2) \le \mu_k (G)$.

114. The general result in **art.** 113 can be sharpened for the specific case of adding one link to a graph. If $G + \{e\}$ is the graph obtained from G by adding a link, then the incidence matrix $B_{G+\{e\}}$ consists of the incidence matrix B_G with one added

column containing the vector z, that has only two non zero elements, 1 at row e^+ and -1 at row e^-. Hence,

$$Q_{G+\{e\}} = B_G B_G^T + zz^T = Q_G + zz^T$$

and

$$\det\left(Q_{G+\{e\}} - \mu I\right) = \det\left(Q_G + zz^T - \mu I\right)$$
$$= \det\left(Q_G - \mu I\right)\det\left(I + \left(Q_G - \mu I\right)^{-1} zz^T\right)$$

Applying the "rank one update" formula (8.82) yields

$$\det\left(I + \left(Q_G - \mu I\right)^{-1} zz^T\right) = 1 + z\left(Q_G - \mu I\right)^{-1} z^T$$

The same argument as in **art. 180** shows that the strictly increasing rational function $\frac{\det\left(Q_{G+\{e\}} - \mu I\right)}{\det\left(Q_G - \mu I\right)}$ only possesses simple poles and zeros that lie in between the poles. From the common zero $\mu_N(G) = \mu_N(G + \{e\}) = 0$ on, the function $\frac{\det\left(Q_{G+\{e\}} - \mu I\right)}{\det\left(Q_G - \mu I\right)}$ increases implying that first the pole at $\mu_{N-1}(G)$ is reached before the zero at $\mu_{N-1}(G + \{e\})$. Hence, we obtain

$$\mu_j(G) \le \mu_j(G + \{e\}) \le \mu_{j-1}(G)$$

for all $1 < i \le N$ and at $i = 1$, $\mu_1(G) \le \mu_1(G + \{e\})$. Comparing this bound for $j = N - 1$ with (4.29) in **art. 95** yields

$$\mu_{N-1}(G) \le \mu_{N-1}(G + \{e\}) \le \min\left(\mu_{N-2}(G), \mu_{N-1}(G) + 2\right)$$

115. *Laplacian spectrum of the cone of a graph.* When a node k is added to a graph G, a similar analysis as in **art. 60** applies. From the adjacency matrix (3.60), the corresponding Laplacian is

$$Q_{(N+1)\times(N+1)} = \begin{bmatrix} Q_{N\times N} + \mathrm{diag}\,(v_i) & -v_{N\times 1} \\ -\left(v^T\right)_{1\times N} & d_k \end{bmatrix}$$

Let us confine ourselves to the special case $v = u$, where the new node k is connected to any other node in graph, thus forming the cone of the graph G. Let w be the eigenvector of $Q_{N\times N}$ belonging to μ_{N-1}, then, for the vector $z^T = \begin{bmatrix} w^T & 0 \end{bmatrix}$,

$$Q_{(N+1)\times(N+1)}z = \begin{bmatrix} Q_{N\times N} + I & -v_{N\times 1} \\ -\left(v^T\right)_{1\times N} & N \end{bmatrix}\begin{bmatrix} w \\ 0 \end{bmatrix} = \begin{bmatrix} \left(\mu_{N-1} + 1\right)w \\ -v^T w \end{bmatrix}$$

Only if $v = u$, in which case $u^T w = 0$, then z is an eigenvalue of $Q_{(N+1)\times(N+1)}$ belonging to $\mu_{N-1} + 1$.

In fact, as shown by Das (2004), the entire spectrum can be deduced by considering the complement G^c_{N+1} of the cone of G_N. Since the cone node has degree N, the complement G^c_{N+1} is disconnected. Theorem 10 states that the Laplacian of G^c_{N+1} has at least two eigenvalues $\mu^c_N = \mu^c_{N-1} = 0$, while **art. 80** tells us that the

remaining Laplacian eigenvalues of G^c_{N+1} are those of G^c_N. Using (4.9) then shows that the set of eigenvalues of the cone of a graph, $\{\mu_j\left(Q_{(N+1)\times(N+1)}\right)\}_{1\leq j\leq N+1}$, are $N+1$, $\mu_j\left(Q_{N\times N}\right)+1$ for $1\leq j\leq N-1$, and zero.

116. *Removal of a node.* Let us consider the graph $G\backslash\{j\}$ obtained by removing an arbitrary node j and its incident links from G. **Art.** 115 shows that the Laplacian eigenvalues of the cone of $G\backslash\{j\}$ equal N, $\mu_1\left(G\backslash\{j\}\right)+1$, $\mu_2\left(G\backslash\{j\}\right)+1$, ..., $\mu_{N-2}\left(G\backslash\{j\}\right)+1$ and 0. The original graph G is a subgraph of the cone of $G\backslash\{j\}$. Since the Laplacian eigenvalues are non decreasing if links are added to the graph (**art.** 113), we conclude that, for all $1\leq j\leq N-2$,

$$\mu_j\left(G\backslash\{j\}\right)+1\geq\mu_{j+1}\left(G\right)$$

117. *Vertex connectivity* $\kappa_{\mathcal{N}}\left(G\right)$. The vertex connectivity of a graph, $\kappa_{\mathcal{N}}\left(G\right)$, is the minimum number of nodes whose removal (together with adjacent links) disconnects the graph G. The Rayleigh principle (**art.** 152) shows, for any other connection vector $v\neq u$ in **art.** 115, that $z^T Q_{(N+1)\times(N+1)}z\geq\mu_{N-1}\left(Q_{(N+1)\times(N+1)}\right)$ such that

$$\mu_{N-1}\left(Q_{(N+1)\times(N+1)}\right)\leq\mu_{N-1}\left(Q_{N\times N}\right)+1$$

Repeating the argument gives

$$\mu_{N-1}\left(Q_{(N+k)\times(N+k)}\right)\leq\mu_{N-1}\left(Q_{N\times N}\right)+k$$

If $\kappa_{\mathcal{N}}\left(G\right)=k$, the above relation shows that

$$\mu_{N-1}\leq\kappa_{\mathcal{N}}\left(G\right)\tag{4.65}$$

Indeed, for a disconnected graph $\mu_{N-1}\left(Q_{N\times N}\right)=0$ and the addition of minimum $\kappa\left(G\right)=k$ nodes connects the graph, i.e., $\mu_{N-1}\left(Q_{(N+k)\times(N+k)}\right)>0$.

118. *Edge connectivity* $\kappa_{\mathcal{L}}\left(G\right)$. The edge connectivity of a graph, $\kappa_{\mathcal{L}}\left(G\right)$, is the minimum number of links whose removal disconnects the graph G. For any connected graph G, it holds that

$$\kappa_{\mathcal{N}}\left(G\right)\leq\kappa_{\mathcal{L}}\left(G\right)\leq d_{\min}(G)\tag{4.66}$$

Indeed, let us concentrate on a connected graph G that is not a complete graph. Since $d_{\min}(G)$ is the minimum degree of a node, say n, in G, by removing all links of node n, G is disconnected. By definition, since $\kappa_{\mathcal{L}}(G)$ is the minimum number of links that leads to disconnectivity, it follows that $\kappa_{\mathcal{L}}(G)\leq d_{\min}(G)$ and $\kappa_{\mathcal{L}}(G)\leq N-2$ because G is not a complete graph and consequently the minimum nodal degree is at most $N-2$. Furthermore, the definition of $\kappa_{\mathcal{L}}(G)$ implies that there exists a set S of $\kappa_{\mathcal{L}}(G)$ links whose removal splits the graph G into two connected subgraphs G_1 and G_2, as illustrated in Fig. 4.2. Any link of that set S connects a node in G_1 to a node in G_2. Indeed, adding an arbitrary link of that set makes G again connected. But G can be disconnected into the same two connected subgraphs by removing nodes in G_1 and/or G_2. Since possible disconnectivity inside

either G_1 or G_2 can occur before $\kappa_{\mathcal{L}}(G)$ nodes are removed, it follows that $\kappa_{\mathcal{N}}(G)$ cannot exceed $\kappa_{\mathcal{L}}(G)$, which establishes the inequality (4.66).
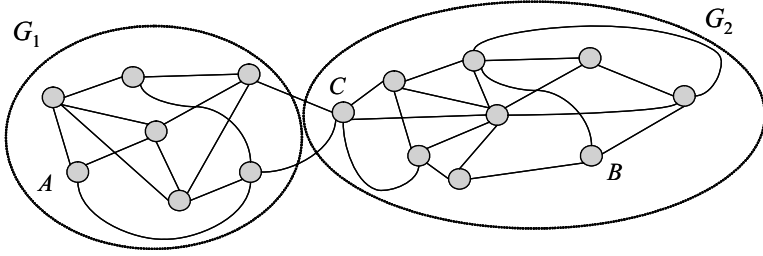

Fig. 4.2. A graph G with $N = 16$ nodes and $L = 32$ links. Two connected subgraphs G_1 and G_2 are shown. The graph's connectivity parameters are $\kappa_{\mathcal{N}}(G) = 1$ (removal of node C), $\kappa_{\mathcal{L}}(G) = 2$ (removal of links from C to G_1), $d_{\min}(G) = 3$ and $E[D] = \frac{2L}{N} = 4$.

Let us proceed to find the number of link disjoint paths between A and B in a connected graph G. Suppose that H is *a* set of links whose removal separates A from B. Thus, the removal of all links in the set H destroys all paths from A to B. The maximum number of link disjoint paths between A and B cannot exceed the number of links in H. However, this property holds for any set H, and thus also for the set with the smallest possible number of links. A similar argument applies to node disjoint paths. Hence, we end up with Theorem 18:

Theorem 18 (Menger's Theorem) *The maximum number of link (node) disjoint paths between A and B is equal to the minimum number of links (nodes) separating (or disconnecting) A and B.*

Recall that the edge connectivity $\kappa_{\mathcal{L}}(G)$ (analogously vertex connectivity $\kappa_{\mathcal{N}}(G)$) is the minimum number of links (nodes) whose removal disconnects G. By Menger's Theorem, it follows that there are at least $\kappa_{\mathcal{L}}(G)$ link disjoint paths and at least $\kappa_{\mathcal{N}}(G)$ node disjoint paths between any pair of nodes in G.

119. *Edge connectivity $\kappa_{\mathcal{L}}(G)$ and the algebraic connectivity μ_{N-1}.* Fiedler (1973) has proved a lower bound for μ_{N-1} in terms of the edge connectivity $\kappa_{\mathcal{L}}(G)$.

Theorem 19 (Fiedler) *For any graph G with L links and N nodes,*

$$\mu_{N-1} \geq 2\kappa_{\mathcal{L}}(G)\left(1 - \cos\frac{\pi}{N}\right) \tag{4.67}$$

Proof: Consider the symmetric, stochastic matrix $P = I - \frac{1}{d_{\max}}Q$ in Theorem 39. The spectral gap of P equals $1 - \lambda_2(P) = \frac{\mu_{N-1}}{d_{\max}}$, and is lower bounded in (8.55) by

$$\psi_n(r(P)) \leq 1 - \lambda_2(P)$$

where $\psi_n(x) = 2x\left(1 - \cos\frac{\pi}{n}\right)$ for $x \leq \frac{1}{2}$ and the measure of irreducibility $r(P)$,

defined in (8.52), equals $r(P) = \frac{\kappa_{\mathcal{L}}(G)}{d_{\max}}$. Indeed, by Merger's Theorem 18, the maximum number of link disjoint paths between node A and B equals the minimum number of links that separates A from B. Hence, there are at least $\kappa_{\mathcal{L}}(G)$ link disjoint paths between any pair of nodes in G. $\qquad\square$

We note that the function $\psi_n(x)$ in Theorem 39 provides a second bound

$$\mu_{N-1} \geq 2\kappa_{\mathcal{L}}(G)\left(\cos\frac{\pi}{N} - \cos\frac{2\pi}{N}\right) - 2d_{\max}\left(1 - \cos\frac{\pi}{N}\right)\cos\frac{\pi}{N}$$

which is only better than (4.67) if and only if $2\kappa_{\mathcal{L}}(G) > d_{\max}$. Using (5.7) for a cir cuit C, shows that $\mu_{N-1}(C) = 2\left(1 - \cos\frac{2\pi}{N}\right)$, while, for a path P, $\mu_{N-1}(P) = 2\left(1 - \cos\frac{\pi}{N}\right)$ follows from (5.8). Also, $\kappa_{\mathcal{L}}(C) = \kappa_{\mathcal{N}}(C) = 2$ and $\kappa_{\mathcal{L}}(P) = \kappa_{\mathcal{N}}(P) = 1$, which shows that equality is achieved in the bound (4.67) for the path P. However, in most cases as verified for example from Fig. 4.1, the lower bound (4.67) is rather weak.

120. *Pendants in a graph.* A node with degree one is called a pendant. Many complex networks possess pendants. If a connected graph G has a pendant, then the second smallest eigenvalue $\mu_{N-1} \leq 1$ as follows from[9] (4.22) in **art. 90**. If the pendant is not adjacent to the highest degree node, then $\mu_{N-1} < 1$. The latter result is based on the observation that, the complement G^c of G, has at least one node of degree $N - 2$, namely the complementary node of the pendant. This node is thus almost the corner node in the cone of G^c and the star tree with this corner node in the center is a spanning tree T if precisely one node at distance 2 of the corner node is added to that star. Since $T = K_{1,N-2} + \{e\}$, **art. 114** shows that

$$\mu_1(T) > \mu_1(K_{1,N-2}) = N - 1$$

because $\mu_1(K_{1,N-2}) = N - 1$ as computed in Section 5.7. Since the spanning tree T is a subtree graph of G^c, **art. 113** implies that

$$\mu_1(G^c) \geq \mu_1(T) > N - 1$$

such that we arrive, with (4.9), at $\mu_{N-1}(G) < 1$.

The following theorem is due to Das (2004):

Theorem 20 (Das) *If G is a connected graph with a Laplacian eigenvalue $0 < \mu < 1$, then the diameter of G is at least 3.*

Proof: Let x denote the eigenvector belonging to μ, then the equation for the j th component is

$$\mu x_j = \sum_{k=1}^{N} q_{jk}x_k = d_j x_j - \sum_{k=1}^{N} a_{jk}x_k = d_j x_j - \sum_{k\in\text{neighbor}(j)} x_k$$

---

[9] Fiedler's general upper bound (4.20) for μ_{N-1} leading to (4.21) is not sharp enough to establish this result.

If $x_j = \max_{1 \leq k \leq N} x_k = x_{\max}$ is the largest component of the eigenvector x and let $x_{\min;j} = \min_{k \in \text{neighbor}(j)} x_k$ with $\arg x_{\min} = k_j$, then

$$x_{\min;j} = (d_j - \mu) x_j - \sum_{k \in \text{neighbor}(j) \backslash k_j}^{N} x_k$$

$$\geq (1 - \mu) x_j$$

because $\sum_{k \in \text{neighbor}(j) \backslash k_j}^{N} x_k \leq (d_j - 1) x_{\max} = (d_j - 1) x_j$.

Similarly, if $x_j = \max_{1 \leq k \leq N} x_k = x_{\min}$ is the largest component of the eigenvector x and let $x_{\max;j} = \max_{k \in \text{neighbor}(j)} x_k$ with $\arg x_{\max} = k_j$, then

$$x_{\max;j} = (d_j - \mu) x_j - \sum_{k \in \text{neighbor}(j) \backslash k_j}^{N} x_k$$

$$\leq (1 - \mu) x_j$$

because $\sum_{k \in \text{neighbor}(j) \backslash k_j}^{N} x_k \geq (d_j - 1) x_{\min} = (d_j - 1) x_j$. These inequalities show that, if $0 < \mu < 1$, the eigenvector components corresponding to the neighbors of the node j with largest (smallest) eigenvector component, have the same sign as x_j. **Art.** 67 shows that the largest and smallest eigenvector component (for $\mu \neq \mu_N = 0$) must have a different sign. This implies that the nodes with largest and smallest eigenvector component are not neighbors (not directly connected), nor have neighbors in common. Since G is connected, this means that the diameter in G is at least 3. $\qquad\square$

5

Spectra of special types of graphs

This chapter presents spectra of graphs that are known in closed form.

5.1 The complete graph

The eigenvalues of the adjacency matrix of the complete graph K_N are $\lambda_1 = N - 1$ and $\lambda_2 = \ldots = \lambda_N = -1$. Since K_N is a regular graph (**art.** 74), the eigenvalues of the Laplacian are, apart from $\mu_N = 0$, all equal to $\mu_j = N$ for $1 \leq j \leq N - 1$.

The eigenvalues can be computed from the determinant in (8.2) in the same way as in **art.** 82. Alternatively, the adjacency matrix of the complete graph is $A_{K_N} = J - I$ and $J = u.u^T$. A direct computation yields

$$\det\left(J - I - \lambda I\right) = \det\left(u.u^T - (\lambda + 1)\,I\right) = \left(-\left(\lambda + 1\right)\right)^N \det\left(I - \frac{u.u^T}{\lambda + 1}\right)$$

Using (8.82) and $u^T u = N$, we obtain

$$\det\left(J - I - \lambda I\right) = \left(-\left(\lambda + 1\right)\right)^N \left(1 - \frac{N}{\lambda + 1}\right)$$

$$= (-1)^N (\lambda + 1)^{N-1} (\lambda + 1 - N)$$

from which the eigenvalues of the adjacency matrix of the complete graph K_N are immediate. In summary,

$$\det\left(J - xI\right)_{n \times n} = (-1)^n x^{n-1} (x - n) \tag{5.1}$$

5.2 A small-world graph

In a small world graph $G_{\mathrm{SW}k}$, each node is placed on a ring as illustrated in Fig. 5.1 and has links to precisely k subsequent neighbors and, by the cyclic structure of the ring, also to k previous neighbors. The small world graph has been proposed by Watts and Strogatz (1998) and is further discussed in Watts (1999) to study the effect of adding random links to a regular network or of rewiring links randomly. The thus modified small world graphs are found to be highly clustered, like regular

graphs. As mentioned in Section 1.3, depending on the rewiring process of links, typical paths may have a large hopcount, unlike in random graphs.

The adjacency matrix $A_{\mathrm{SW}k}$ is of the type of a symmetric circulant, Toeplitz matrix whose eigenvalue structure (eigenvalues and eigenvectors) can be exactly determined by the Fourier matrix.
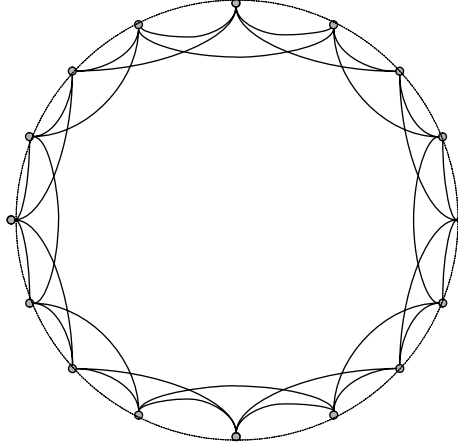

Fig. 5.1. A Watts Strogatz small world graph $G_{\mathrm{SW}k}$ with $k = 2$ is a regular graph with degree $d = 4$.

5.2.1 The eigenvalue structure of a circulant matrix

A circulant matrix C is an $n \times n$ matrix with the form

$$C = \begin{pmatrix} c_0 & c_{n-1} & c_{n-2} & \cdots & c_1 \\ c_1 & c_0 & c_{n-1} & \cdots & c_2 \\ c_2 & c_1 & c_0 & \ddots & c_3 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ c_{n-1} & c_{n-2} & c_{n-3} & \cdots & c_0 \end{pmatrix}$$

Each column is precisely the same as the previous one, but the elements are shifted one position down and wrapped around at the bottom. In fact, $c_{jk} = c_{(j-k) \bmod n}$, which shows that diagonals parallel to the main diagonal contain the same elements. The elementary circulant matrix E has all zero elements except for $c_1 = 1$,

$$E = \begin{pmatrix} 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

and represents a unit shift relabeling transformation of nodes: $1 \to 2, 2 \to 3, \ldots, n \to 1$. Thus, the unit shift relabeling transformation, which is a particular example of a permutation (**art.** 10), maps the vector $x = (x_1, x_2, \ldots, x_n)$ into $Ex = (x_n, x_1, x_2, \ldots, x_{n-1})$. Again applying the unit shift relabeling transformation maps Ex into $E^2 x = (x_{n-1}, x_n, x_1, \ldots, x_{n-2})$, which is a two shift relabeling transformation, and

$$E^2 = \begin{pmatrix} 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 & 0 & 0 \end{pmatrix}$$

Hence, we observe that E^2 equals the circulant matrix C with all $c_j = 0$, except for $c_2 = 1$. In general, E^k represents a k shift relabeling transformation, where each node label $n_j \to n_{(j+k) \bmod n}$ and E^k equals C with all $c_j = 0$, except for $c_k = 1$. Alternatively, a general circulant matrix C can be decomposed into elementary k shift relabeling matrices E^k (where $E^0 = I$) as

$$C = c_0 I + c_1 E + c_2 E^2 + c_{n-1} E^{n-1} = \sum_{k=0}^{n-1} c_k E^k$$

Denoting the polynomial $p(x) = \sum_{k=0}^{n-1} c_k x^k$, we can write that $C = p(E)$. The eigenstructure of E can be found quite elegantly. Indeed, $Ex = \lambda x$ is equivalent to solving the set, for both λ and all components x_k of x,

$$x_n = \lambda x_1$$
$$x_1 = \lambda x_2$$
$$x_2 = \lambda x_3$$
$$\vdots$$
$$x_{n-1} = \lambda x_n$$

After multiplying all equations, we find $\prod_{j=1}^{n} x_j = \lambda^n \prod_{j=1}^{n} x_j$, from which $\lambda^n = 1$ and $\lambda_k = e^{\frac{2\pi i k}{n}}$, for $k = 0, 1, \ldots, n-1$. The roots of unity $\lambda_k = e^{\frac{2\pi i k}{n}}$ obey $\lambda_k^* = e^{-\frac{2\pi i k}{n}}$, $\lambda_k^* \lambda_k = |\lambda_k|^2 = 1$ and, thus with (8.6) in **art.** 138, we obtain $\det E = \prod_{k=0}^{n-1} \lambda_k = (-1)^{n-1}$. Any eigenvector is only determined apart from a scaling factor, we may choose $x_1 = \alpha$ and, after backsubstitution in the set, we find that $x_k = \lambda^{1-k} \alpha$ for all $k = 1, \ldots, n-1$ and $x_n = \lambda = \lambda^{1-n}$ because $\lambda^n = 1$. Thus, the eigenvector of E belonging to the eigenvalue λ_k equals $\alpha \left(1, \lambda_k^{-1}, \lambda_k^{-2}, \ldots, \lambda_k^{-n+1}\right)$ and the matrix X containing the eigenvectors of E as column vectors is, with

$\xi = e^{-\frac{2\pi i}{n}}$,

$$X = \alpha \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \xi & \xi^2 & \cdots & \xi^{n-1} \\ 1 & \xi^2 & \xi^4 & \cdots & \xi^{n-2} \\ \vdots & \vdots & \vdots & & \\ 1 & \xi^{n-1} & \xi^{n-2} & \cdots & \xi \end{pmatrix}$$

where $(X)_{kj} = \xi^{-(k-1)(j-1)}$. We observe that $X^T = X$. If x and y are the eigenvectors belonging to eigenvalue λ_k and λ_j, respectively, then the inner product $x^H y$ (**art.** 150) is

$$x^H y = \sum_{l=1}^{n} x_l^* y_l = \alpha^2 \sum_{l=1}^{n} \left(\lambda_k^{1-l}\right)^* \lambda_j^{1-l} = \alpha^2 e^{\frac{2\pi i(j-k)}{n}} \sum_{l=1}^{n} \left(e^{-\frac{2\pi i(j-k)}{n}}\right)^l$$

$$= \alpha^2 \sum_{l=0}^{n-1} \left(e^{-\frac{2\pi i(j-k)}{n}}\right)^l = \alpha^2 \frac{1 - e^{-2\pi i(j-k)}}{1 - e^{-\frac{2\pi i(j-k)}{n}}}$$

Since $e^{2\pi i m} = 1$ for any integer m, we have that $x^H y = 0$ if $k \neq j$, and $x^H y = n\alpha^2$ if $k = j$ which suggests the normalization $\alpha^2 n = 1$. Hence, with $\alpha = \frac{1}{\sqrt{n}}$, we have shown that X is a unitary matrix (**art.** 151), that obeys $X^H X = X X^H = I$. The matrix X is also called the Fourier matrix. The eigenvalue equation, written in terms of the matrix X, is $EX = X\Lambda$, where

$$\Lambda = \text{diag}\left(1, e^{\frac{2\pi i}{n}}, e^{\frac{4\pi i}{n}}, \ldots, e^{\frac{2\pi i k}{n}}, \ldots, e^{\frac{2\pi i(n-1)}{n}}\right)$$

$$= \text{diag}\left(1, \xi^{-1}, \xi^{-2}, \ldots, \xi^{-(n-1)}\right)$$

Using the unitary property results, after left multiplication of both sides by X^H, in

$$X^H E X = \text{diag}\left(1, \xi^{-1}, \xi^{-2}, \ldots, \xi^{-(n-1)}\right)$$

and

$$X^H E^k X = \text{diag}\left(1, \xi^{-k}, \xi^{-2k}, \ldots, \xi^{-(n-1)k}\right)$$

Since $\det E \neq 0$, the inverse E^{-1} exists and is found as

$$E^{-1} = X \text{diag}\left(1, \xi, \xi^2, \ldots, \xi^{(n-1)}\right) X^H$$

Explicitly,

$$\left(E^{-1}\right)_{kj} = \frac{1}{n} \sum_{m=1}^{n} (X)_{km} \xi^{m-1} (X^H)_{mj} = \frac{1}{n} \sum_{m=1}^{n} \xi^{-(k-1)(m-1)+(m-1)-(m-1)(j-1)}$$

$$= \frac{1}{n} \sum_{m=0}^{n-1} e^{-\frac{2\pi i(k-j+1)}{n} m}$$

$$= \frac{1}{n} \frac{1 - e^{-2\pi i(k-j+1)}}{1 - e^{-\frac{2\pi i(k-j+1)}{n}}} = 1_{\{k=j-1\}}$$

Thus, $E^{-1} = E^{n-1}$, which corresponds to a unit shift relabeling transformation in the other direction: $1 \to n,\ 2 \to 1,\ldots,\ n \to n-1$.

Finally, the eigenvalue structure of a general circulant matrix $C = p(E) = \sum_{k=0}^{n-1} c_k E^k$ is

$$
X^H C X = X^H \left(\sum_{k=0}^{n-1} c_k E^k \right) X = \sum_{k=0}^{n-1} c_k X^H E^k X
$$

$$
= \sum_{k=0}^{n-1} c_k \, \mathrm{diag}\left(1, \xi^{-k}, \xi^{-2k}, \ldots, \xi^{-(n-1)k} \right)
$$

$$
= \mathrm{diag}\left(\sum_{k=0}^{n-1} c_k,\ \sum_{k=0}^{n-1} c_k \xi^{-k},\ \sum_{k=0}^{n-1} c_k \xi^{-2k},\ \ldots,\ \sum_{k=0}^{n-1} c_k \xi^{-(n-1)k} \right)
$$

In terms of the polynomial $p(x)$, we arrive at the eigenvalue decomposition of a general circulant matrix C,

$$
X^H C X = \mathrm{diag}\left(p(1), p\left(\xi^{-1}\right), p\left(\xi^{-2}\right), \ldots, p\left(\xi^{-(n-1)}\right) \right) \tag{5.2}
$$

5.2.2 The spectrum of a small-world graph

The adjacency matrix $A_{\mathrm{SW}k}$ of a small world graph where each node, placed on a ring, has links to precisely k subsequent and k previous neighbors, is a symmetric circulant matrix where $c_{N-j} = c_j$ (symmetry) and $c_0 = 0$, $c_j = 1_{\{j \in [1,k]\}}$, where 1_y is the indicator function. Since the degree of each node is $2k$ and the maximum possible degree is $N-1$, the value of k is limited to $2k+1 \le N$. The corresponding polynomial is denoted as $p_{\mathrm{SW}k}(z) = \sum_{j=0}^{N-1} c_j z^j$. Since $c_0 = 0$, we have that

$$
p_{\mathrm{SW}k}(z) = \sum_{j=1}^{N-1} c_j z^j = \sum_{j=1}^{a} c_j z^j + \sum_{j=a+1}^{N-1} c_j z^j
$$

$$
= \sum_{j=1}^{a} c_j z^j + \sum_{j=1}^{N-a-1} c_{N-j} z^{N-j}
$$

By symmetry $c_{N-j} = c_j$, the last sum is, for any integer $a \in [1, N-1]$,

$$
p_{\mathrm{SW}k}(z) = \sum_{j=1}^{a} c_j z^j + \sum_{j=1}^{N-a-1} c_j z^{N-j}
$$

When choosing $a = k$, the bound $2k+1 \le N$ implies that $N - a - 1 = N - k - 1 \ge k$. Invoking $c_j = 1_{\{j \in [1,k]\}}$ and with $a = k$, we obtain

$$
p_{\mathrm{SW}k}(z) = \sum_{j=1}^{k} z^j + z^N \sum_{j=1}^{k} z^{-j}
$$

$$
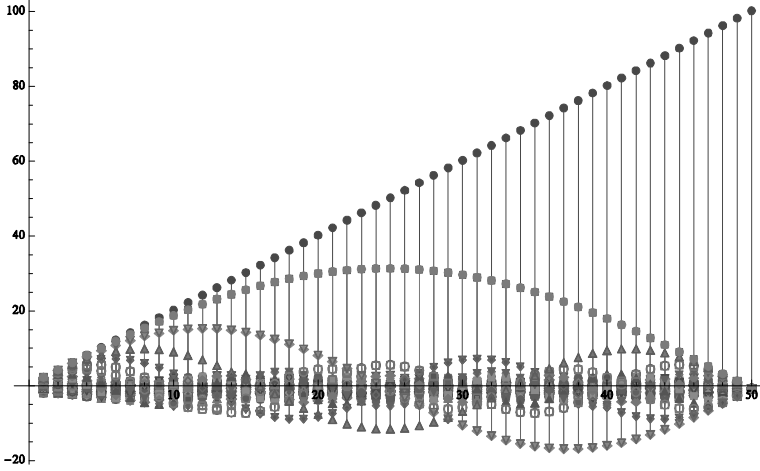= z \frac{1 - z^k}{1 - z} + z^{N-1} \frac{1 - z^{-k}}{1 - z^{-1}}
$$

Fig. 5.2. The complete spectrum (5.3) for $N = 101$. The x axis plots all values of k from 1 to $\left[\frac{n-1}{2}\right] = 50$, and for each k, all $1 \leq m \leq N$ values of $(\lambda_{\mathrm{SW}\,k})_m$ are shown.

The spectrum of $A_{\mathrm{SW}\,k}$ follows for $m = 1, \ldots, N$ from (5.2) as

$$
(\lambda_{\mathrm{SW}\,k})_m = p_{\mathrm{SW}\,k}\left(\xi^{1-m}\right) = \xi^{1-m}\frac{1 - \xi^{(1-m)k}}{1 - \xi^{1-m}} + \xi^{(1-m)(N-1)}\frac{1 - \xi^{(m-1)k}}{1 - \xi^{m-1}}
$$

$$
= e^{\frac{2\pi i}{N}(m-1)}\frac{1 - e^{\frac{2\pi i}{N}(m-1)k}}{1 - e^{\frac{2\pi i}{N}(m-1)}} + e^{-\frac{2\pi i}{N}(m-1)}\frac{1 - e^{-\frac{2\pi i}{N}(m-1)k}}{1 - e^{-\frac{2\pi i}{N}(m-1)}}
$$

$$
= 2\,\mathrm{Re}\left(e^{\frac{2\pi i}{N}(m-1)}\frac{1 - e^{\frac{2\pi i}{N}(m-1)k}}{1 - e^{\frac{2\pi i}{N}(m-1)}}\right)
$$

After rewriting

$$
\frac{1 - e^{\frac{2\pi i}{N}(m-1)k}}{1 - e^{\frac{2\pi i}{N}(m-1)}} = e^{\frac{\pi i}{N}(m-1)(k-1)}\frac{\sin\left(\frac{\pi(m-1)k}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}
$$

the eigenvalue with index m of $A_{\mathrm{SW}\,k}$ is

$$
(\lambda_{\mathrm{SW}\,k})_m = 2\,\mathrm{Re}\left(\frac{e^{\frac{\pi i}{N}(m-1)(k+1)}\sin\left(\frac{\pi(m-1)k}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}\right)
$$

$$
= 2\frac{\sin\left(\frac{\pi(m-1)k}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}\cos\left(\frac{\pi(m-1)(k+1)}{N}\right)
$$

$$
= \frac{-\sin\left(\frac{\pi(m-1)}{N}\right) + \sin\left(\frac{\pi(m-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}
$$

Finally, the unordered[1] eigenvalues of $A_{\mathrm{SW}\,k}$ are, for $1 \leq m \leq N$,

$$(\lambda_{\mathrm{SW}\,k})_m = \frac{\sin\left(\frac{\pi(m-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)} - 1 \tag{5.3}$$

The complete spectrum for $N = 101$ is drawn in Fig. 5.2, which is representative for values of N roughly above 50. Fig. 5.2 illustrates the spectral evolution (as function of k in the abscissa) from a circuit ($k = 1$) towards the complete graph ($k = \left[\frac{N-1}{2}\right]$).

Applying $\sin(x + n\pi) = (-1)^n \sin(x)$, valid for any integer n, we find additional symmetry in the eigenvalue spectrum,

$$(\lambda_{\mathrm{SW}\,k})_m = \frac{\sin\left(\frac{\pi(2k+1)\{N-(m-1)\}}{N}\right)}{\sin\left(\frac{\pi\{N-(m-1)\}}{N}\right)} - 1 = (\lambda_{\mathrm{SW}\,k})_{N+2-m}$$

for $2 \leq m \leq N$. In general, we cannot deduce more symmetry because, if N is a prime, precisely $\left[\frac{N}{2} + 1\right]$ eigenvalues are distinct for any $k < \frac{N-1}{2}$. Theorem 5 states that the diameter of $G_{\mathrm{SW}\,k}$ is at most $\left[\frac{N}{2}\right]$ when N is prime. Fig. 5.3 reflects the irregular dependence of the number of different eigenvalues, which reminds us of the irregular structure of quantities in number theory, such as the number of divisors and the prime number factorization.

The Chebyshev polynomial of the second kind (Abramowitz and Stegun, 1968, Sections 22.3.7, 22.3.16), defined by

$$U_n(z) = \frac{\sin(n+1)\arccos z}{\sin \arccos z} = \sum_{k=0}^{\left[\frac{n}{2}\right]}(-1)^k \frac{(n-k)!}{k!(n-2k)!}(2z)^{n-2k} \tag{5.4}$$

has zeros at $z_m = \cos\frac{m\pi}{n+1}$ for $m = 1, \ldots, n$ such that

$$U_n(z) = 2^n \prod_{m=1}^{n}\left(z - \cos\frac{m\pi}{n+1}\right) \tag{5.5}$$

In terms of the Chebyshev polynomial of the second kind, we can write (5.3) as

$$(\lambda_{\mathrm{SW}\,k})_m = U_{2k}\left(\cos\left(\frac{\pi(m-1)}{N}\right)\right) - 1$$

For example, if $m = 1$ in (5.3), then $(\lambda_{\mathrm{SW}\,k})_1 = 2k$. We know that $(\lambda_{\mathrm{SW}\,k})_1$ is the largest eigenvalue because, for a regular graph, the maximum eigenvalue equals the degree (**art.** 41). Also, if $2k + 1 = N$ in which case $A_{\mathrm{SW}\,k} = J - I$, then we obtain from (5.3)

$$\lim_{2k+1 \to N}(\lambda_{\mathrm{SW}\,k})_j = -1$$

---

[1] The m-th ordered eigenvalue $(\lambda_{\mathrm{SW}\,k})_{(m)}$, satisfying $(\lambda_{\mathrm{SW}\,k})_{(m)} \geq (\lambda_{\mathrm{SW}\,k})_{(m+1)}$, for $1 \leq m < N$, is not easy to determine as Fig. 5.2 suggests.
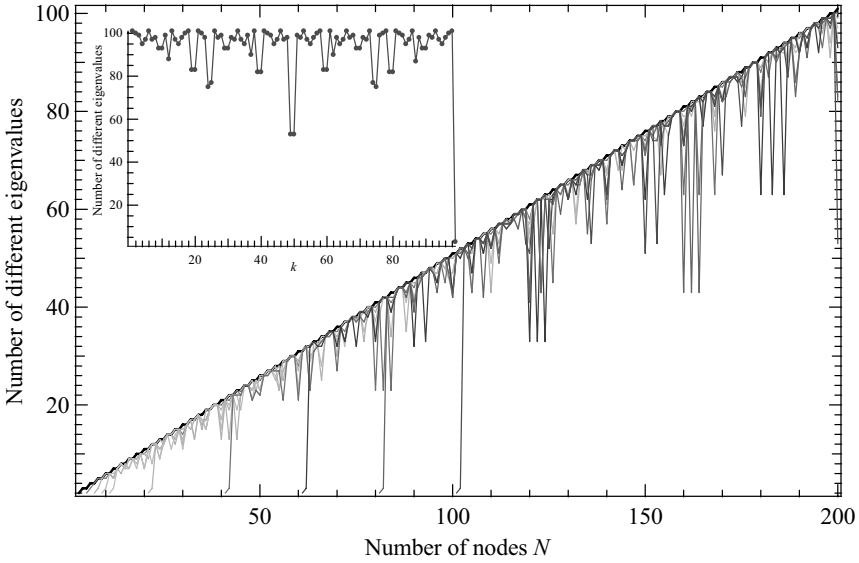
Fig. 5.3. The number of different eigenvalues in $A_{\mathrm{SW}k}$ as a function of N for different values of $k = 1, 2, 3, 4, 5$ and $k = 10, 20, 30, 40, 50$. The insert shows the number of different eigenvalues for $N = 200$ versus k.

for all $m \neq 1$, while $(\lambda_{\mathrm{SW}k})_1 = N-1$. Of course, this spectrum corresponds to that of the complete graph K_N, derived in Section 5.1. Since a small world graph is a regular graph (**art.** 74), the Laplacian $Q_{\mathrm{SW}k} = 2kI - A_{\mathrm{SW}k}$ and the corresponding unordered spectrum is

$$(\mu_{\mathrm{SW}k})_{N+1-m} = 2k - (\lambda_{\mathrm{SW}k})_m$$

$$= 2k + 1 - \frac{\sin\left(\frac{\pi(m-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}$$

As Theorem 10 prescribes, there is precisely one zero eigenvalue $(\mu_{\mathrm{SW}k})_N = 0$. **Art.** 74 demonstrates that $(\mu_{\mathrm{SW}k})_{N-1}$ equals the spectral gap, the difference between the largest and second largest eigenvalue at each k as illustrated in Fig. 5.2.

The largest negative eigenvalue of $(\lambda_{\mathrm{SW}k})_m$ lies between $\frac{N}{2k+1} < m - 1 < \frac{2N}{2k+1}$ (and, by symmetry $m \to N + 2 - m$, $\frac{2kN}{2k+1} > m - 1 > \frac{(2k-1)N}{2k+1}$). Indeed, if we let $x = \frac{\pi(m-1)}{N}$ and $x \in [0, \pi)$, then the function $f(x) = \frac{\sin(2k+1)x}{\sin x} - 1$ has the same derivative as $\tilde{f}(x) = \frac{\sin(2k+1)x}{\sin x}$, which has zeros at $x = \frac{l\pi}{2k+1} \in [0, \pi)$ for $l = 1, 2, \ldots, 2k$. By Rolle's Theorem, $f'(x)$ has always a zero in an interval between two zeros of $f(x)$ since $f(x)$ is continuous. Since $\sin x$ has the same sign in $x \in (0, \pi)$, the largest absolute values of $f(x)$ will occur near $x \to 0$ and $x \to \pi$, where $\sin x$ has zeros. A good estimate for the value at which the largest

negative eigenvalue occurs is half of the interval, hence, $m_{\min} = \left[\frac{3N}{2(2k+1)} + 1 \right]$. The corresponding eigenvalue is, approximately,

$$(\lambda_{\mathrm{SW}\,k})_{m_{\min}} \approx - \frac{1}{\sin\left(\frac{3\pi}{2(2k+1)} \right)} - 1 < -2$$

Numerical values indicate that $m_{\min} = \left[\frac{3N}{2(2k+1)} + 1 \right]$ is, in many cases, exact. Hence, the eigenvalues $\lambda_{\mathrm{SW}\,k}$ of the adjacency matrix A_{SW_k} lie in the interval $\left[(\lambda_{\mathrm{SW}\,k})_{m_{\min}}, 2k \right]$, and most of them lie in the interval $\left[(\lambda_{\mathrm{SW}\,k})_{m_{\min}}, 0 \right]$. This interval is, to a good approximation, independent of the size of the graph N, but only a function of the degree of each node, which is $2k$. The approximation fails for the complete graph K_N when $2k + 1 = N$ (and thus odd) and $(\lambda_{\mathrm{SW}\,k})_{m_{\min}} = -1$.

5.3 A circuit on N nodes

A circuit C is a ring topology where each node on a circle is connected to its previous and subsequent neighbor on the ring. Hence, the circuit is a special case of the small world graph for $k = 1$. The adjacency matrix of the circuit is thus $A_C = E + E^{-1}$. The eigenvalues of the circuit follow directly from (5.3) as

$$(\lambda_C)_m = \frac{\sin\left(3\frac{\pi(m-1)}{N} \right)}{\sin\left(\frac{\pi(m-1)}{N} \right)} - 1$$

Using the identities $\sin 3x = 3 \sin x - 4 \sin^3 x$ and $1 - 2 \sin^2 x = \cos 2x$ yields, for $m = 1, \ldots, N$,

$$(\lambda_C)_m = 2 \cos\left(\frac{2\pi(m-1)}{N} \right) \tag{5.6}$$

which shows that $(\lambda_C)_m = (\lambda_C)_{N-m+2}$ and that $-2 \le (\lambda_C)_m \le 2$. The lower bound of -2 is only attained for N is even. We notice that the line graph of the circuit is the circuit itself: $l(C) = C$. Since the number of links $L = N$ in the circuit C, the prefactor $(\lambda + 2)^{L-N}$ in the general expression (2.9) of the characteristic polynomial of a line graph vanishes. Nevertheless, only if N is even, this line graph $l(C)$ still has an eigenvalue equal to -2, while all other eigenvalues are larger (**art. 9**).

The corresponding Laplacian spectrum follows from **art. 74** as

$$(\mu_C)_{N+1-m} = 2 - 2 \cos\left(\frac{2\pi(m-1)}{N} \right) \qquad m = 1, \ldots, N \tag{5.7}$$

The characteristic polynomial of the circuit C is

$$c_C(\lambda) = \prod_{m=1}^{N} \left(2 \cos\left(\frac{2\pi(m-1)}{N} \right) - \lambda \right) = \prod_{m=1}^{N} \left(2 \cos\left(\frac{2\pi m}{N} \right) - \lambda \right)$$

where the last equality follows from the symmetry relation $(\lambda_C)_m = (\lambda_C)_{N-m}$. The

zeros of the Chebyshev polynomial $T_n(z)$ of the first kind (Abramowitz and Stegun, 1968, Sections 22.3.6, 22.3.15), defined by

$$T_n(z) = \cos(n \arccos z) = \frac{n}{2} \sum_{k=0}^{\left[\frac{n}{2}\right]} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!} (2z)^{n-2k}$$

are $z_m = \cos\left(\frac{\pi(2m-1)}{2n}\right)$ for $m = 1, \ldots, n$, from which the product form

$$T_n(z) = 2^{n-1} \prod_{m=1}^{n} \left(z - \cos\left(\frac{\pi(2m-1)}{2n}\right)\right)$$

follows. On the other hand, the zeros of $\cos(n \arccos z) - 1 = 0$ are $z_m = \cos\left(\frac{2m\pi}{n}\right)$, for $m = 1, \ldots, n$. Thus,

$$c_C(\lambda) = \prod_{m=1}^{N} \left(2\cos\left(\frac{2\pi m}{N}\right) - \lambda\right) = 2^N \prod_{m=1}^{N} \left(\cos\left(\frac{2\pi m}{N}\right) - \frac{\lambda}{2}\right)$$

and, in terms of the Chebyshev polynomial $T_n(x)$ of the first kind,

$$c_C(\lambda) = 2(-1)^N \left(T_N\left(\frac{\lambda}{2}\right) - 1\right)$$

5.4 A path of $N-1$ hops

A path consisting of $N-1$ hops has an adjacency matrix A_P where each row has precisely one non zero element in the upper triangular part. There exists a relabeling transformation that transforms the adjacency matrix A_P of the path (line) on N nodes in a tri diagonal Toeplitz matrix, where each non zero element appears on the line parallel and just above the main diagonal. The eigenstructure of the general $N \times N$ tri diagonal Toeplitz matrix,

$$T = \begin{bmatrix} b & a & & & \\ c & b & a & & \\ & \ddots & \ddots & \ddots & \\ & & c & b & a \\ & & & c & b \end{bmatrix}$$

is computed in Van Mieghem (2006b, Section A.5.2.1). The matrix T has N distinct eigenvalues λ_m, for $1 \leq m \leq N$,

$$\lambda_m = b + 2\sqrt{ac} \cos\left(\frac{\pi m}{N+1}\right)$$

The components $(x_m)_k$ of the eigenvector x_m belonging to λ_m are, for $1 \leq k \leq N$,

$$(x_m)_k = 2\alpha \left(\frac{c}{a}\right)^{\frac{k}{2}} \sin\left(\frac{\pi mk}{N+1}\right)$$

Since the eigenvalues are invariant under a similarity transform such as a relabeling transformation (**art.** 142), the complete eigenvalue and eigenvector system of A_P follows, for $a = c = 1$ and $b = 0$, from the eigenstructure of the general $N \times N$ tri diagonal Toeplitz matrix for $m = 1, \ldots N$, as

$$(\lambda_P)_m = 2 \cos \left(\frac{\pi m}{N + 1} \right) \tag{5.8}$$

Formula (5.8) shows that $(\lambda_P)_m = -(\lambda_P)_{N+1\ m}$ and that all eigenvalues of the $N - 1$ hops path P are strictly smaller than 2, in particular, $-2 < (\lambda_P)_m < 2$. The largest eigenvalue of the path P is the smallest largest adjacency eigenvalue among any connected graph as proved by Lovász and Pelikán (1973). We provide another reasoning: Lemma 7 shows that a tree has the smallest λ_1, because it is the connected graph with the minimum number of links. Further, the tree with minimum maximum degree ($d_{\max} = 2$) and minimum degree variance is the path. According to the bound (3.45) and $L = N - 1$ in any tree, the bounds for the largest eigenvalue of the path satisfies

$$2 \left(1 - \frac{1}{N} \right) \le 2 \sqrt{1 - \frac{6}{N}} \le \lambda_1 (P) \le 2$$

and the lower bound even tends to the upper bound for large N. Any other tree has a larger variance, thus a larger lower bound in (3.45), while also the upper bound is larger than $d_{\max} > 2$.

The characteristic polynomial of the path is

$$c_P (\lambda) = \prod_{m=1}^{N} \left(2 \cos \left(\frac{\pi m}{N + 1} \right) - \lambda \right) = (-1)^N U_N \left(\frac{\lambda}{2} \right)$$

where the Chebyshev polynomial $U_N (x)$ of the second kind (5.5) has been used.

After a suitable relabeling (as above), the Laplacian Q_P of an $N - 1$ hops path is, except for the first and last row, a Toeplitz matrix,

$$Q_P = \begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix}$$

We compute here the eigenstructure of Q_P analogous to the derivation of the eigenstructure of the general $N \times N$ tri diagonal Toeplitz matrix in Van Mieghem (2006b, Section A.5.2.1). An eigenvector x corresponding to eigenvalue μ satisfies

$(Q - \mu I)\, x = 0$ or, written per component,

$$(1 - \mu)x_1 - x_2 = 0$$
$$-x_{k\,1} + (2 - \mu)x_k - x_{k+1} = 0 \qquad\qquad 2 \le k \le N - 1$$
$$-x_{N\,1} + (1 - \mu)x_N = 0$$

Consider the generating function $G(z) = \sum_{k=1}^{N} x_k z^k$, where all x_k are real because all eigenvalues μ of the Laplacian are real. **Art.** 67 demonstrates that $G(1) = 0$ when the eigenvector $x \ne \alpha u$, else the eigenvector αu, where α is a suitable normalization, belongs to the $\mu = 0$ eigenvalue and $G(z) = \alpha \sum_{k=1}^{N} z^k = z\frac{1}{1}\frac{z^{N+1}}{z}$ and $G(1) = \alpha N$.

After multiplying the k th vector component equation by z^k and summing over all $k \in [2, N-1]$, the above difference equation is transformed into

$$z \sum_{k=1}^{N\,2} x_k z^k + (\mu - 2) \sum_{k=2}^{N\,1} x_k z^k + z^{\,1} \sum_{k=3}^{N} x_k z^k = 0$$

and, in terms of $G(z)$,

$$z\left(G(z) - x_{N\,1}z^{N\,1} - x_N z^N\right) + (\mu - 2)\left(G(z) - x_1 z - x_N z^N\right) + \frac{G(z) - x_2 z^2 - x_1 z}{z} = 0$$

Thus,

$$\left(z^2 + (\mu - 2)z + 1\right) G(z) = x_{N\,1}z^{N+1} + x_N z^{N+2} + (\mu - 2)x_1 z^2$$
$$+ (\mu - 2)x_N z^{N+1} + x_2 z^2 + x_1 z$$
$$= (z - 1)\, z \left(x_N z^N - x_1\right)$$

where in the last step the first and last vector component equation has been used. Solving for $G(z)$ yields

$$G(z) = \frac{(z - 1)\, z \left(x_N z^N - x_1\right)}{z^2 + (\mu - 2)z + 1}$$
$$= \frac{x_N (z - 1)\, z \left(z^N - \frac{x_1}{x_N}\right)}{(z - r_1)(z - r_2)}$$

where r_1 and r_2 are the roots of the polynomial $z^2 + (\mu - 2)z + 1 = 0$, thus obeying $r_1 + r_2 = 2 - \mu$ and $r_1 r_2 = 1$. Since $G(z)$ is a polynomial of order N, the zeros r_1 and r_2 must also be zeros of $(z - 1)\, z \left(z^N - \frac{x_1}{x_N}\right)$. Thus, r_1 and r_2 must be either 0, 1 or $\left(\frac{x_1}{x_N}\right)^{1/N} e^{\frac{2\pi i m}{N}}$ for $m = 0, 1, \ldots, N - 1$. Since $r_1 r_2 = 1$, neither r_1 nor r_2 can be zero. If $r_1 = 1$, then also $r_2 = 1$ in which case $\mu = 0$ and $x_1 = x_N$ as follows by raising $\left(\frac{x_1}{x_N}\right)^{1/N} e^{\frac{2\pi i m}{N}} = 1$ to the power N. In that case, $G(z) = \frac{x_N z(z^N\,1)}{(z\,1)} = x_N \sum_{k=1}^{N} z^k$ such that the corresponding eigenvector is, indeed, the scaled all one vector αu with $\alpha = x_N$. All positive eigenvalues $\mu > 0$

correspond to distinct zeros $r_1 = \left(\frac{x_1}{x_N}\right)^{1/N} e^{\frac{2\pi i m}{N}}$ for $m = 0, 1, 2, \ldots, N-1$. But, since $r_2 = r_1^{-1}$, the zero r_2 also must be of this form, $r_2 = \left(\frac{x_1}{x_N}\right)^{1/N} e^{\frac{2\pi i n}{N}}$ for some $0 \le n \ne m \le N-1$. Thus, the product

$$r_1 r_2 = \left(\frac{x_1}{x_N}\right)^{2/N} e^{\frac{2\pi i (m+n)}{N}} = 1$$

raised to the power N, shows that $\frac{x_1}{x_N} = \pm 1 = e^{i\pi k}$ such that $r_1 = e^{\frac{\pi i (2m+k)}{N}}$ and $r_2 = e^{\frac{\pi i (2n+k)}{N}}$. Requiring that $r_2 = r_1^{-1}$ results in $r_1 = e^{\frac{\pi i (m-n)}{N}}$ and $r_2 = e^{\frac{\pi i (n-m)}{N}} = e^{-\frac{\pi i (m-n)}{N}}$. Now, r_1 changes with m, while r_2 with n. For each $m = 1, 2, \ldots, N-1$, there must correspond to $l = m - n$ in the exponent of r_1, a value $-l = -(m-n)$ in r_2, only by changing $n \ne m$, thus $n = m - l$. The extent over which the integer l can range is $-(N-1) \le l \le N-1$ and to each l there must correspond a $-l$. Hence, for $l = 1, 2, \ldots, N-1$, we finally find that

$$\mu_l = 2 - (r_1 + r_2) = 2 - \left(e^{\frac{\pi i l}{N}} + e^{-\frac{\pi i l}{N}}\right)$$

$$= 2\left(1 - \cos\left(\frac{\pi l}{N}\right)\right) = 4\sin^2 \frac{\pi l}{2N}$$

and to $l = 0$, the case $r_1 = r_2 = 1$ corresponds with $\mu_0 = 0$. In summary, the *ordered* Laplacian eigenvalues of the $N-1$ hops path are

$$(\mu_P)_{N-m} = 2\left(1 - \cos\left(\frac{\pi m}{N}\right)\right) \qquad m = 0, 1, \ldots, N-1 \qquad (5.9)$$

All Laplacian eigenvalues of the path are simple, while most of the circuit Laplacian eigenvalues in (5.7) have double multiplicity.

We now determine the eigenvectors $x_1, x_2, \ldots, x_{N-1}$ and use the notation $(x_m)_j$ for the j th component of the eigenvector x_m. The eigenvector x_m corresponding to $\mu_m = (\mu_P)_{N-m} > 0$ has the generating function $G_m(z) = \sum_{k=1}^{N} (x_m)_k z^k$, which equals

$$G_m(z) = \frac{(x_m)_N (z-1) z \left(z^N - \frac{(x_m)_1}{(x_m)_N}\right)}{\left(z - e^{\frac{\pi i m}{N}}\right)\left(z - e^{-\frac{\pi i m}{N}}\right)}$$

Invoking **art. 210** to the polynomial

$$p_0(z) = (x_m)_N (z-1) z \left(z^N - \frac{(x_m)_1}{(x_m)_N}\right)$$

which is written as

$$p_0(z) = \sum_{j=0}^{N+2} a_j z^j = (x_m)_N z^{N+2} - (x_m)_N z^{N+1} - (x_m)_1 z^2 + (x_m)_1 z$$

yields

$$G_m(z) = \frac{1}{e^{\frac{\pi i m}{N}} - e^{\frac{\pi i m}{N}}} \sum_{k=0}^{N} \left\{ \sum_{j=k+1}^{N+2} a_j \left(e^{(j\ k\ 1)\frac{\pi i m}{N}} - e^{(j\ k\ 1)\frac{\pi i m}{N}} \right) \right\} z^k$$

$$= \frac{1}{\sin \frac{\pi m}{N}} \sum_{k=0}^{N} \left\{ \sum_{j=k+1}^{N+2} a_j \sin \left(\frac{\pi m}{N}(j-k-1) \right) \right\} z^k$$

from which, for $0 \le k \le N$,

$$(x_m)_k = \frac{1}{\sin \frac{\pi m}{N}} \sum_{j=k+1}^{N+2} a_j \sin \left(\frac{\pi m}{N}(j-k-1) \right)$$

Since $(x_m)_0 = 0$, this component relation reduces to

$$0 = \sum_{j=1}^{N+2} a_j \sin \left(\frac{\pi m}{N}(j-1) \right) = (x_m)_N \sin \left(\frac{\pi m}{N}(N+1) \right) - (x_m)_1 \sin \left(\frac{\pi m}{N} \right)$$

such that

$$(x_m)_N = (-1)^m (x_m)_1$$

For $k > 0$, we have that

$$(x_m)_k = \frac{1}{\sin \frac{\pi m}{N}} \sum_{j=k+2}^{N+2} a_j \sin \left(\frac{\pi m}{N}(j-k-1) \right)$$

$$= \frac{(x_m)_N}{\sin \frac{\pi m}{N}} \left\{ \sin \left(\frac{\pi m}{N}(N-k+1) \right) - \sin \left(\frac{\pi m}{N}(N-k) \right) \right\}$$

$$= \frac{2(x_m)_N}{\sin \frac{\pi m}{N}} \sin \left(\frac{\pi m}{2N} \right) \cos \left(\frac{\pi m}{2N}(2N-2k+1) \right)$$

Using $(x_m)_N = (-1)^m (x_m)_1$, we finally find the k th component of the eigenvector x_m belonging to the eigenvalue $\mu_m = (\mu_P)_{N\ m} > 0$,

$$(x_m)_k = \frac{(x_m)_1}{\cos \frac{\pi m}{2N}} \cos \left(\frac{\pi m}{2N}(2k-1) \right)$$

A proper normalization of the eigenvectors, obeying $x_k^T x_m = \delta_{km}$ as in **art. 151**, is readily obtained for $1 \le m \le N-1$ as

$$(x_m)_k = \sqrt{\frac{2}{N}} \cos \frac{\pi m}{2N}(2k-1) \text{ for } 1 \le k \le N$$

Obviously, the eigenvector $x_N = \frac{u}{\sqrt{N}}$ belonging to $\mu_N = 0$ has the components

$$(x_N)_j = \frac{1}{\sqrt{N}} \text{ for } 1 \le j \le N$$

5.5 A path of h hops

A path of $h > 0$ hops/links in a graph with N nodes has h non zero rows with one non zero element in the upper triangular part. After a similarity transform, the corresponding adjacency matrix can be transformed into

$$A_{h\text{-hop path}} = \begin{bmatrix} (A_P)_{(h+1)\times(h+1)} & O_{(h+1)\times(N\ h\ 1)} \\ O_{(N\ h\ 1)\times(h+1)} & O_{(N\ h\ 1)\times(N\ h\ 1)} \end{bmatrix}$$

where A_P is the tri diagonal Toeplitz adjacency matrix of an h hops path in a graph with $h + 1$ nodes. Invoking (5.8), the spectrum of an h hops path possesses a zero eigenvalue of multiplicity $N - h - 1$ and $h + 1$ eigenvalues

$$(\lambda_{h\text{-hop path}})_k = 2\cos\left(\frac{\pi k}{h+2}\right)$$

for $k = 1, \ldots, h + 1$.

5.6 The wheel W_{N+1}

The wheel graph W_{N+1} is the graph obtained by adding to the circuit graph one central node n with links (spokes) to each node of the circuit. Thus, the wheel graph is the cone of the circuit graph. The adjacency matrix is a special case of **art. 60**,

$$A_W = \begin{bmatrix} A_C & u_{N\times 1} \\ u_{1\times N} & 0 \end{bmatrix}$$

Since u is an eigenvector of A_C belonging to $\lambda_C = 2$ because the circuit is a regular graph, all eigenvalues of A_C are the same as those of $A_{W_{N+1}}$, except for the largest eigenvalue $\lambda_C = 2$, which is replaced by two new ones, $1 \pm \sqrt{1 + N}$, as derived in **art. 60**. Hence, the spectrum of the wheel with $N + 1$ nodes is $-\sqrt{1 + N} + 1$, $\left\{2\cos\left(\frac{2\pi(m\ 1)}{N}\right)\right\}_{2\leq m \leq N}$ and $1 + \sqrt{1 + N}$.

The Laplacian spectrum follows from **art. 115** and (5.7) as, $(\mu_W)_{N+1} = 0$, $(\mu_W)_1 = N + 1$ and

$$(\mu_W)_{N+2\ m} = 3 - 2\cos\left(\frac{2\pi(m-1)}{N}\right) \qquad m = 2, \ldots, N$$

5.7 The complete bipartite graph $K_{m,n}$

The complete bipartite graph $K_{m,n}$ consists of two sets $\mathcal{M}$ and $\mathcal{N}$ with $m = |\mathcal{M}|$ and $n = |\mathcal{N}|$ nodes respectively, where each node of one set is connected to all other nodes of the other set. There are no links between nodes of a same set. The adjacency matrix of $K_{m,n}$ is, with $N = m + n$,

$$A_{K_{m,n}} = \begin{bmatrix} O_{m\times m} & J_{m\times n} \\ J_{n\times m} & O_{n\times n} \end{bmatrix}$$

and the characteristic polynomial is

$$\det\left(A_{K_{m,n}} - \lambda I\right) = \begin{bmatrix} -\lambda I_{m\times m} & J_{m\times n} \\ J_{n\times m} & -\lambda I_{n\times n} \end{bmatrix}$$

Invoking (8.79) and $J_{k\times n}J_{n\times l} = nJ_{k\times l}$ gives

$$\det\left(A_{K_{m,n}} - \lambda I\right) = (-\lambda)^m \det\left(-\lambda I_{n\times n} + \frac{1}{\lambda}J_{n\times m}J_{m\times n}\right)$$
$$= (-\lambda)^m \det\left(\frac{m}{\lambda}J - \lambda I\right)_{n\times n}$$
$$= (-\lambda)^m \left(\frac{m}{\lambda}\right)^n \det\left(J - \frac{\lambda^2}{m}I\right)_{n\times n}$$

Using (5.1), the characteristic polynomial of $K_{m,n}$ is

$$\det\left(A_{K_{m,n}} - \lambda I\right) = (-\lambda)^m \left(\frac{m}{\lambda}\right)^n (-1)^{n-1}\left(\frac{\lambda^2}{m}\right)^{n-1}\left(\frac{\lambda^2}{m} - n\right)$$
$$= (-1)^{m+n-1}\lambda^{m+n-2}\left(\lambda^2 - mn\right)$$

from which the eigenvalues[2] follow as $-\lambda_{\max}, [0]^{N-2}$ and $\lambda_{\max} = \sqrt{mn}$. This spec trum reduces to that of a star topology $K_{1,n}$ for $m = 1$.

The Laplacian of the complete bipartite graph $K_{m,n}$ is

$$Q_{K_{m,n}} = \begin{bmatrix} nI_{m\times m} & -J_{m\times n} \\ -J_{n\times m} & mI_{n\times n} \end{bmatrix}$$

and the characteristic polynomial is

$$\det\left(Q_{K_{m,n}} - \mu I\right) = \begin{bmatrix} (n-\mu)I_{m\times m} & -J_{m\times n} \\ -J_{n\times m} & (m-\mu)I_{n\times n} \end{bmatrix}$$

A derivation similar to the above results in

$$\det\left(Q_{K_{m,n}} - \mu I\right) = -(m-\mu)^{n-1}(n-\mu)^{m-1}\left((m-\mu)(n-\mu) - nm\right)$$

The eigenvalues of $Q_{K_{m,n}}$ are $0, [m]^{n-1}, [n]^{m-1}$ and $m+n = N$. In the case of the star $K_{1,n}$, the eigenvalues of $Q_{K_{1,n}}$ are $0, [1]^{n-1}$ and $n+1$. The complexity $\xi(N)$, the number of trees in $K_{m,n}$, is found from (4.14) as

$$\xi_{K_{m,n}}(N) = \frac{1}{N}\prod_{k=1}^{N-1}\mu_k = m^{n-1}n^{m-1}$$

and clearly, for the star where $m = 1$, $\xi_{K_{1,n}}(N) = 1$.

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[2] We denote the multiplicity m of an eigenvalue λ by $[\lambda]^m$

5.8 A general bipartite graph

5.8.1 Undirected bipartite graph

Instead of connecting each of the $m \leq n$ nodes in the set $\mathcal{M}$ to each of the n nodes in the other set $\mathcal{N}$, we may consider an arbitrary linking between the two sets represented by a matrix $R_{m \times n}$, resulting in a general bipartite graph $B_{m,n}$ with adjacency matrix

$$A_{B_{m,n}} = \begin{bmatrix} O_{m \times m} & R_{m \times n} \\ R_{n \times m}^T & O_{n \times n} \end{bmatrix}$$

Using (8.80) when $m \leq n$, the characteristic polynomial is

$$\det\left(A_{B_{m,n}} - \lambda I\right) = (-\lambda)^n \det\left(-\lambda I_{m \times m} + \frac{1}{\lambda} R_{m \times n} R_{n \times m}^T\right)$$

$$= (-\lambda)^{n-m} \det\left(R_{m \times n} R_{n \times m}^T - \lambda^2 I_{m \times m}\right)$$

while, using (8.79) when $m > n$, we obtain

$$\det\left(A_{B_{m,n}} - \lambda I\right) = (-\lambda)^{m-n} \det\left(R_{n \times m}^T R_{m \times n} - \lambda^2 I_{n \times n}\right)$$

These two forms for $m \leq n$ and $m > n$ are an illustration of Lemma 10. In the sequel, we confine to the case where $m \leq n$ without loss of generality.

The singular value decomposition of R is $R = U_{m \times m} \left(\Sigma_R\right)_{m \times n} V_{n \times n}^T$, where $\Sigma_R = \mathrm{diag}(\sigma_1, \ldots, \sigma_m, 0, \ldots, 0)$, because the rank of R cannot be larger than $m \leq n$ and where U and V are orthonormal matrices (**art. 151**). From $UU^T = I$ and $RR^T = U_{m \times m} \Sigma_{m \times m}^2 U_{m \times m}^T$, we see that

$$\det\left(R_{m \times n} R_{n \times m}^T - \lambda^2 I_{m \times m}\right) = \det\left(U_{m \times m} \left(\Sigma_{m \times m}^2 - \lambda^2 I\right) U_{m \times m}^T\right)$$

$$= \prod_{j=1}^{m} \left(\sigma_j^2 - \lambda^2\right)$$

Hence, the spectrum of the general bipartite graph is

$$\det\left(A_{B_{m,n}} - \lambda I\right) = (-1)^{m-n} \lambda^{n-m} \prod_{j=1}^{m} \left(\sigma_j^2 - \lambda^2\right)$$

which show that, apart from the zero eigenvalues, it is completely determined by the singular values of R, because $\lambda = \pm \sigma_j$ for $j = 1, \ldots, m$.

Since

$$A_{B_{m,n}}^2 = \begin{bmatrix} R_{m \times n} R_{n \times m}^T & O_{m \times n} \\ O_{n \times m} & R_{n \times m}^T R_{m \times n} \end{bmatrix}$$

and, further for any integer $k \geq 1$, that

$$A_{B_{m,n}}^{2k} = \begin{bmatrix} \left(R_{m \times n} R_{n \times m}^T\right)^k & O_{m \times n} \\ O_{n \times m} & \left(R_{n \times m}^T R_{m \times n}\right)^k \end{bmatrix}$$

and

$$A_{B_{m,n}}^{2k+1} = \left[\begin{array}{cc} O_{m \times m} & \left(R_{m \times n}R_{n \times m}^{T}\right)^{k} R_{m \times n} \\ \left(R_{n \times m}^{T}R_{m \times n}\right)^{k} R_{n \times m}^{T} & O_{n \times n} \end{array} \right]$$

the even powers $A_{B_{m,n}}^{2k}$ are reducible non negative matrices (**art.** 167), while the odd powers again represent a "bipartite" matrix structure.

5.8.2 Directed bipartite graph

A general *directed* bipartite graph BG has an adjacency matrix,

$$A_{BG} = \left[\begin{array}{cc} O_{m \times m} & B_{m \times n} \\ C_{n \times m} & O_{n \times n} \end{array} \right] \tag{5.10}$$

Any tree T on $N = n + m$ nodes can be represented in the form of a levelset. Denote by $\left\{X_N^{(k)}\right\}$ the k th level set of a tree T, which is the set of nodes in the tree T at hopcount k from the root in a graph with N nodes, and by $X_N^{(k)}$ the number of elements in the set $\left\{X_N^{(k)}\right\}$. Then, we have $X_N^{(0)} = 1$ because the zeroth level can only contain the root node itself. For all $k > 0$, it holds that $0 \leq X_N^{(k)} \leq N - 1$ and that

$$\sum_{k=0}^{N-1} X_N^{(k)} = N \tag{5.11}$$

Nodes $X_N^{(k)}$ at a same level k are not interconnected. Fig. 5.4 draws a tree organized per level.
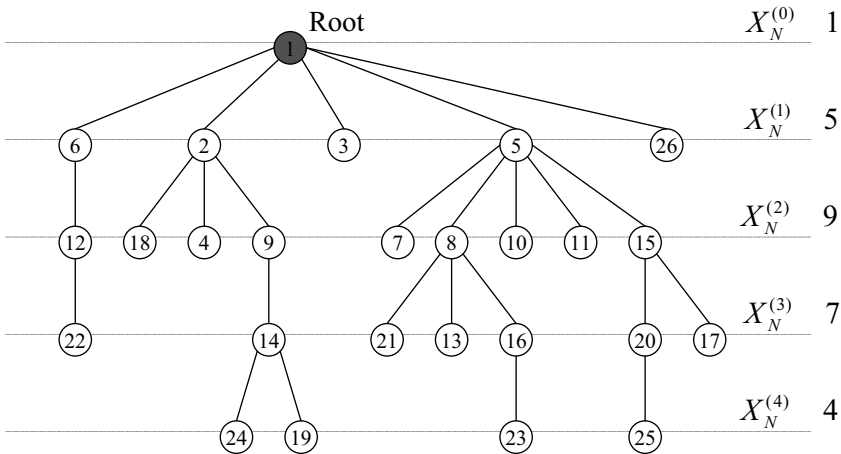

Fig. 5.4. An instance of a tree with $N = 26$ nodes organized per level $0 \leq k \leq 4$. The nodes in the tree are arbitrarily labeled.

The levelset can be folded level by level to form a general bipartite graph. Indeed, the root connects to the nodes $X_N^{(1)}$ at hop 1; those $X_N^{(1)}$ are the ancestors of all the nodes on levelset $X_N^{(2)}$. We may arrange these $X_N^{(2)}$ nodes at the side of the root. Next, these $X_N^{(2)}$ are the ancestors of all $X_N^{(3)}$ nodes, which we move to the other side of the $X_N^{(1)}$ node. In this way, all even levels are placed at the side of the root and all odd levels at the other side, thus creating a general directed bipartite graph. Hence, *the adjacency matrix of any tree can be recast in the form of (5.10),* where $m = \sum_{k=0}^{\frac{N-1}{2}} X_N^{(2k)}$ and $n = \sum_{k=0}^{\frac{N-2}{2}} X_N^{(2k+1)} = N - m$. In a stochastic setting, where $E\left[X_N^{(k)}\right] = N \Pr\left[H_N = k\right]$, we observe that the average multiplicity of the zero eigenvalue equals (assuming $n > m$)

$$E\left[n - m\right] = N \sum_{k=0}^{N-1} \Pr\left[H_N = k\right] (-1)^k = N \varphi_{H_N}(-1)$$

where the probability generating function of the hopcount in a random tree is $\varphi_{H_N}(z) = E\left[z^{H_N}\right] = \sum_{k=0}^{N-1} \Pr\left[H_N = k\right] z^k$.

If $x^T = \begin{bmatrix} x_C & x_B \end{bmatrix}^T$ is an eigenvector belonging to eigenvalue λ, which means that

$$\begin{bmatrix} O_{m \times m} & B_{m \times n} \\ C_{n \times m} & O_{n \times n} \end{bmatrix} \begin{bmatrix} x_{C_{m \times 1}} \\ x_{B_{n \times 1}} \end{bmatrix} = \begin{bmatrix} B x_B \\ C x_C \end{bmatrix} = \begin{bmatrix} \lambda x_C \\ \lambda x_B \end{bmatrix}$$

then also $x^T = \begin{bmatrix} x_C & -x_B \end{bmatrix}^T$ is an eigenvector belonging to the eigenvalue $-\lambda$, which shows that the spectrum is symmetric around $\lambda = 0$. The same result can be derived from (8.79) analogously to the spectrum of $A_{B_{m,n}}$ above as

$$\det\left(A_{BG} - \lambda I\right) = (-1)^{m-n} \lambda^{n-m} \det\left(B_{m \times n} C_{n \times m} - \lambda^2 I_{m \times m}\right)$$

Hence, A_{BG} has, at least, $n - m$ zero eigenvalues. Consequently, we have demonstrated:

Theorem 21 *The spectrum of the adjacency matrix of any tree is symmetric around $\lambda = 0$ with $n - m$ zero eigenvalues.*

5.8.3 Symmetry in the spectrum of an adjacency matrix A

Theorem 21 can also be proven as follows. If the spectrum of A is symmetric, the characteristic polynomial $c_A(x) = c_A(-x)$ is even, which implies that the odd coefficients c_{2k+1} of the characteristic polynomial $c_A(x)$ are all zero. **Art. 29** shows that the product $a_{1p_1} a_{2p_2} \ldots a_{kp_k}$ of a permutation $p = (p_1, p_2, \ldots, p_k)$ of $(1, 2, \ldots, k)$ in a tree is always zero for odd k. Hence, (3.4) indicates that the spectrum of the adjacency matrix of any tree is symmetric. Indeed, the only non zero product $a_{1p_1} a_{2p_2} \ldots a_{kp_k}$ in a tree is obtained when a link is traversed in both directions. Loops longer than two hops are not possible due to the tree structure and the permutation requirement for the determinant. The latter only admits paths of

k hops as subgraphs G_k in **art. 29** because all first as well as second indices need to different in $a_{1p_1} a_{2p_2} \ldots a_{kp_k}$ (since $a_{jj} = 0$). A longer (even) loop containing more than two hops will visit the intermediate nodes of the k hop path twice, which the determinant structure does not allow.

The skewness s_λ, defined in **art. 36**, is zero for a tree, which again agrees with Theorem 21.

We have called the spectrum of a matrix A symmetric around $\lambda = 0$ when, for each eigenvalue $\lambda = r > 0$ of A, there is an eigenvalue $\lambda = -r$ of A. The reverse of Theorem 21 is:

Theorem 22 *If the spectrum of an adjacency matrix A is symmetric around $\lambda = 0$, then the corresponding graph is a bipartite graph.*

Proof: Consider the adjacency matrix

$$A = \begin{bmatrix} O_{m \times m} & B_{m \times n} \\ C_{n \times m} & D_{n \times n} \end{bmatrix}$$

where $C = B^T$ if the graph is undirected. Any adjacency matrix can be written in this form for $m \geq 1$, because $a_{jj} = 0$. The characteristic polynomial $\det (A - \lambda I)$ follows from (8.79) as

$$\det (A - \lambda I) = (-\lambda)^{m-n} \det \left(\lambda D_{n \times n} - \lambda^2 I_{n \times n} - C_{n \times m} B_{m \times n} \right)$$

The determinant on the right hand side is only a symmetric polynomial in λ if $D = O$. In that case, A equals the adjacency matrix (5.10) of a bipartite graph. □

5.8.4 Laplacian spectrum of a tree

We have shown in Section 5.8.2 that any tree can be represented by a general bipartite graph after properly folding the levelsets. **Art. 7** indicates that the unsigned incidence matrix R and the incidence matrix B satisfy $B^T B = R^T R$, provided the links are directed from a node at an even levelset $X_N^{(2k)}$ to a node at an odd levelset $X_N^{(2k+1)}$ (or all in the opposite direction), for all levels $0 \leq k < N - 1$. Under this condition, the relation (2.10) in **art. 9** applies such that, with $L = N - 1$ in any tree T,

$$\mu_j (T) = \lambda_j \left(A_{l(T)} \right) + 2 \tag{5.12}$$

for $1 \leq j < N$ and $\mu_N (T) = 0$, as for any graph. Hence, the j th Laplacian eigenvalue of a tree T equals the j th eigenvalue of the $(N - 1) \times (N - 1)$ adjacency matrix of its corresponding line graph $l(T)$.

Petrović and Gutman (2002) have elegantly proven that the path (with $N - 1$ hops) is the tree with smallest largest Laplacian eigenvalue. Their arguments are as follows. When adding a link to a graph, the Laplacian eigenvalues are non decreasing as shown in **art. 114** such that, among all connected graphs, some tree

will have the smallest largest Laplacian, because a tree has the minimum number of links of any connected graph. Now, (5.12) shows that the smallest largest Laplacian in any tree is attained in the tree whose line graph has the smallest largest adjacency eigenvalue. This line graph has $N - 1$ nodes. The line graph of any tree on $N > 4$ nodes possesses cycles, except for the path P_N (of $N - 1$ hops). Any connected cycle containing graph G on $N - 1$ nodes has a spanning tree that contains the minimum number of links and whose largest adjacency eigenvalue is smaller than $\lambda_1 (G)$ by Lemma 7. As shown in Section 5.4, the path P_{N-1} has the smallest largest adjacency eigenvalue among all trees on $N - 1$ nodes. Since the line graph of the path P_N is the path P_{N-1}, we conclude that the path P_N has the smallest largest Laplacian eigenvalue among connected graphs. Combining (5.8) for P_{N-1} and (5.12) yields

$$\mu_1 (P_N) = 2 \left(1 + \cos \left(\frac{\pi}{N}\right)\right) < 4$$

which agrees, indeed, with (5.9).

5.9 Complete multi-partite graph

Instead of two partitions, we now consider the complete m partite graph, where each partition of k_j nodes with $1 \leq j \leq m$ is internally not connected, but fully connected to any other partition. The corresponding adjacency matrix is

$$A_{m\text{-partite}} = \begin{bmatrix} O_{k_1} & J_{k_1 \times k_2} & \cdots & J_{k_1 \times k_m} \\ J_{k_2 \times k_1} & O_{k_2} & \cdots & J_{k_2 \times k_m} \\ \vdots & & \ddots & \vdots \\ J_{k_m \times k_1} & \cdots & \cdots & O_{k_m} \end{bmatrix}$$

The complement of the m partite graph is the union of m cliques $K_{k_1}, K_{k_2}, \ldots, K_{k_m}$, whose spectrum is the union of the eigenvalues of each clique, given by (5.1). Thus, the eigenvalues of $A^c_{m\text{-partite}}$ are $\{k_j - 1\}_{1 \leq j \leq m}$ and $[-1]^{N-m}$, where $N = \sum_{j=1}^{m} k_j$. As we will see below, but also from **art. 40**, the eigenvalues of $A^c_{m\text{-partite}}$ are not quite helpful to derive those of $A_{m\text{-partite}}$.

If all $k_j = k$, then $A_{m\text{-partite}} = A_{K_m} \otimes J_{k \times k}$, whose corresponding spectrum follows from **art. 185** as $\{\lambda_j (A_{K_m}) \lambda_l (J_{k \times k})\}_{1 \leq j \leq m, 1 \leq l \leq k}$, where, according to (5.1), $\lambda_j (A_{K_m}) \in \{m - 1, [-1]^{m-1}\}$ and $\lambda_l (J_{k \times k}) \in \{k, [0]^{k-1}\}$. Thus, when all $k_j = k$ and $N = km$, the eigenvalues of $A_{m\text{-partite}}$ are $(m - 1) k, [0]^{N-m}$ and $[-k]^{m-1}$.

The general case is obtained using the quotient matrix (**art. 15**). Since the row sum of each block matrix in $A_{m\text{-partite}}$ is the same, the partition is equitable, with

corresponding quotient matrix

$$(A^\pi)_{m\text{-partite}} = \begin{bmatrix} 0 & k_2 & \cdots & k_m \\ k_1 & 0 & \cdots & k_m \\ \vdots & & \ddots & \vdots \\ k_1 & k_2 & \cdots & 0 \end{bmatrix} = (J - I)_m \operatorname{diag}(k_j)$$

The eigenvalues of $(A^\pi)_{m\text{-partite}}$ are the non trivial eigenvalues of $A_{m\text{-partite}}$. The remaining $N - m$ eigenvalues of $A_{m\text{-partite}}$ are zero, because, only when $\lambda = 0$, the matrix $A_{m\text{-partite}} - \lambda I$ has in each block k_j identical rows.

The eigenvalues of $(A^\pi)_{m\text{-partite}}$ are obtained by subtracting the first row from all the others, which results in

$$\det\left((A^\pi)_{m\text{-partite}} - \lambda I\right) = \begin{bmatrix} -\lambda & k_2 & k_3 & \cdots & k_m \\ k_1 + \lambda & -(\lambda + k_2) & 0 & \cdots & 0 \\ k_1 + \lambda & 0 & -(\lambda + k_3) & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ k_1 + \lambda & 0 & 0 & \cdots & -(\lambda + k_m) \end{bmatrix}$$

$$= \begin{bmatrix} -\lambda & y^T \\ (k_1 + \lambda)u & \operatorname{diag}(-(\lambda + k_j)) \end{bmatrix}$$

where the $(m-1) \times 1$ vector $y = (k_2, k_3, \ldots, k_m)$. Using the Schur complement (8.80),

$$\det\left((A^\pi)_{m\text{-partite}} - \lambda I\right) = (-1)^m \prod_{j=2}^m (\lambda + k_j) \det\left(\lambda + y^T \operatorname{diag}\left(\frac{-1}{\lambda + k_j}\right)(k_1 + \lambda)u\right)$$

$$= (-1)^m \prod_{j=2}^m (\lambda + k_j)\left(\lambda - (k_1 + \lambda)\sum_{j=2}^m \frac{k_j}{\lambda + k_j}\right)$$

and the eigenvalues are the zeros of the polynomial of degree m in λ

$$\det\left((A^\pi)_{m\text{-partite}} - \lambda I\right) = (-1)^m \left(\lambda \prod_{j=2}^m (\lambda + k_j) - \sum_{l=2}^m k_l \prod_{j=1; j\neq l}^m (\lambda + k_j)\right)$$

When multiplying out, we find that all coefficients c_j of the polynomial

$$\det\left((A^\pi)_{m\text{-partite}} - \lambda I\right) = (-1)^{m-1} \sum_{j=0}^m c_j \lambda^j$$

are positive, except for $c_m = -1$ and $c_{m-1} = 0$. Explicitly, we have

$$c_0 = (-1)^{m-1} \det\left((A^\pi)_{m\text{-partite}}\right) = (m-1) \prod_{j=1}^m k_j$$

and

$$c_j = (m - j - 1) e_{m-j}(k_1, k_2, \ldots, k_n)$$

for $0 \leq j \leq m - 2$, where e_k is the elementary symmetric polynomial (**art. 200**). **Art.** 218 demonstrates that $\det\left((A^{\pi})_{m\text{-partite}} - \lambda I\right)$ has only one positive zero, while all others are negative. The positive zero the largest eigenvalue of $A_{m\text{-partite}}$ and $(A^{\pi})_{m\text{-partite}}$ is the unique, positive solution of

$$\sum_{j=1}^{m} \frac{1}{1 + \frac{\lambda}{k_j}} = 1 \tag{5.13}$$

which shows that $(m-1)\min_{1\leq j\leq m} k_j \leq \lambda \leq (m-1)\max_{1\leq j\leq m} k_j$.

The spectral gap of $A_{m\text{-partite}}$ is equal to the largest eigenvalue of $(A^{\pi})_{m\text{-partite}}$, because $\lambda_2\left(A_{m\text{-partite}}\right) = 0$. Therefore, an explicit expression for the the largest eigenvalue $\lambda_1\left(A_{m\text{-partite}}\right)$ is desirable to estimate the influence of the partitions k_j on the spectral gap. Below, we devote some effort and present two different expansions for $\lambda_1\left(A_{m\text{-partite}}\right)$. If all $k_j = k$, then, as found above,

$$\det\left((A^{\pi})_{m\text{-partite}} - \lambda I\right) = (-1)^m (\lambda + k)^{m-1} (\lambda - (m-1)k)$$

which reduces to the characteristic polynomial (5.1) of the complete graph K_m if $k = 1$. The spectral gap is $km - k = N - k$, which equals that of the complete graph K_N minus k. When not all k_j are equal, the spectral gap is smaller than $N - k$ as verified from Lagrange optimization of (5.13) for all k_j subject to $N = \sum_{j=1}^{m} k_j$. This underlines that regularity in a graph's structure scores highest in terms of robustness.

The Lagrange expansion (**art. 234**) of the zero $\zeta(z_0) = \lambda_1\left(A_{m\text{-partite}}\right)$ of

$$f(z) = \sum_{j=1}^{m} \frac{1}{1 + \frac{z}{k_j}} - 1$$

around z_0, where $z_0 \geq (m-1)\min_{1\leq j\leq m} k_j$, follows from (9.42) in which

$$\frac{f_0(z_0)}{f_1(z_0)} = \frac{1 - \sum_{j=1}^{m} \frac{k_j}{k_j + z_0}}{\sum_{j=1}^{m} \frac{k_j}{(k_j + z_0)^2}}$$

and, for any integer $q > 0$,

$$\frac{f_q(z_0)}{f_1(z_0)} = \frac{(-1)^{q-1} \sum_{j=1}^{m} \frac{k_j}{(k_j + z_0)^{q+1}}}{\sum_{j=1}^{m} \frac{k_j}{(k_j + z_0)^2}}$$

Clearly, the closer z_0 is chosen to $\lambda_1\left(A_{m\text{-partite}}\right)$, the smaller $\frac{f_0(z_0)}{f_1(z_0)}$ and the faster the Lagrange series (9.42) converges (because $\left|\frac{f_q(z_0)}{f_1(z_0)}\right| < 1$ for any $q > 1$ and $z_0 \geq 0$). A reasonable choice is $z_0 = N$, although $z_0 = \frac{m-1}{m}N$ is better as deduced below. Since the Lagrange series (9.42) up to five terms lacks elegance and insight with these $\frac{f_q(z_0)}{f_1(z_0)}$, we present another method.

We can rewrite (5.13) as

$$\lambda = \frac{m-1}{\sum_{j=1}^{m} \frac{1}{\lambda+k_j}} \tag{5.14}$$

from which $\lambda > \frac{m-1}{\sum_{j=1}^{m} \frac{1}{k_j}}$. Iterating (5.14) once gives a sharper lower bound

$$\lambda > \frac{m-1}{\sum_{j_1=1}^{m} \frac{1}{k_{j_1} + \frac{m-1}{\sum_{j_2=1}^{m} \frac{1}{k_{j_2}}}}} = \frac{m-1}{\left(\sum_{j_2=1}^{m} \frac{1}{k_{j_2}}\right)\left(\sum_{j_1=1}^{m} \frac{1}{1+\sum_{j_2=1}^{m} \frac{k_{j_1}}{k_{j_2}}}\right)}$$

After q times iterating the equation, we obtain a finite continued fraction expansion

$$\lambda > \frac{m-1}{\sum_{j_1=1}^{m} \frac{1}{k_{j_1} + \frac{m-1}{\sum_{j_2=1}^{m} \frac{1}{k_{j_2} + \frac{m-1}{\ddots \frac{m-1}{\sum_{j_q=1}^{m} \frac{1}{k_{j_q}}}}}}}}$$

that approaches $\lambda_1 (A_{m\text{-partite}})$ arbitrarily close from below for sufficiently large q.

Finally, for real positive numbers $a_1, a_2, \ldots, a_n$, the harmonic, geometric and arithmetic mean inequality (Hardy *et al.*, 1999) is

$$\frac{n}{\sum_{j=1}^{n} \frac{1}{a_j}} \leq \sqrt[n]{\prod_{j=1}^{n} a_j} \leq \frac{1}{n}\sum_{j=1}^{n} a_j \tag{5.15}$$

with equality only if all a_j are equal. Applied to (5.14) yields

$$\lambda = \frac{m-1}{m}\frac{m}{\sum_{j=1}^{m} \frac{1}{\lambda+k_j}} \leq \frac{m-1}{m}\frac{1}{m}\left(\sum_{j=1}^{m}\lambda + \sum_{j=1}^{m}k_j\right) = \frac{m-1}{m}\left(\lambda + \frac{N}{m}\right)$$

whence

$$\lambda \leq \frac{m-1}{m}N$$

Only when $m = N$ (in case $k_j = 1$), the largest eigenvalue $\lambda_1 (A_{m\text{-partite}})$ equals that of the complete graph.

5.10 An m-fully meshed star topology

In the complete bipartite graph $K_{m,n}$, the m star nodes are not interconnected among themselves. The opposite variant, which we now consider, is essentially $K_{m,n}$ where all nodes in the m set are fully connected. We denote this topology by $G_{m\text{star}}$. The adjacency matrix of a graph of m stars, in which node 1 up to node m has degree $N-1$ while all other nodes have degree m, is

$$A_{m\text{star}} = \begin{bmatrix} (J-I)_{m\times m} & J_{m\times(N-m)} \\ J_{(N-m)\times m} & O_{(N-m)\times(N-m)} \end{bmatrix}$$

Observe that $A_{mstar} = A_{K_{m,n}} + \check{A}_{K_m}$, where

$$\check{A}_{K_m} = \begin{bmatrix} (J-I)_{m\times m} & O_{m\times(N\ m)} \\ O_{(N\ m)\times m} & O_{(N\ m)\times(N\ m)} \end{bmatrix}$$

The characteristic polynomial is

$$\det\left(A_{mstar} - \lambda I\right) = \det \begin{bmatrix} (J-(\lambda+1)\,I)_{m\times m} & J_{m\times(N\ m)} \\ J_{(N\ m)\times m} & -\lambda I_{(N\ m)\times(N\ m)} \end{bmatrix}$$

and this determinant will be solved in two ways by applying (8.79) first and then (8.80).

Applying (8.79) and using

$$X_{m\times m} = (J-(\lambda+1)\,I)_{m\times m} \tag{5.16}$$

gives

$$\det\left(A_{mstar} - \lambda I\right) = \det\left(X\right)\det\left(-\lambda I - J_{(N\ m)\times m}X_{m\times m}^{\ 1}J_{m\times(N\ m)}\right)$$

We first need to compute the inverse of $X_{m\times m} = (J-(\lambda+1)\,I)_{m\times m}$, which we compute as $X^{\ 1} = \frac{\text{adj}X}{\det X}$, where the adjoint matrix adj(A) is the transpose of the matrix of the cofactors of A. An inspection of the matrix X shows that there are precisely two types of cofactors. The cofactor $\mathring{X}_{jj}$ of a diagonal element of X equals

$$\mathring{X}_{jj} = \det \begin{bmatrix} -\lambda & 1 & \cdots & 1 \\ 1 & -\lambda & \cdots & 1 \\ \vdots & & \ddots & \vdots \\ 1 & 1 & \cdots & -\lambda \end{bmatrix} = \det\left(J-(\lambda+1)I\right)_{(m\ 1)\times(m\ 1)}$$

The off diagonal cofactor $\mathring{X}_{ij}$ (with $i \neq j$) is

$$\mathring{X}_{ij} = (-1)^{i+j}\det \begin{bmatrix} & & & \overset{i\text{-th col}}{} & & \\ -\lambda & 1 & \cdots & 1 & \cdots & 1 \\ 1 & -\lambda & \cdots & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 & \cdots & -\lambda \end{bmatrix}$$

where the j th row and the i th column consist of all ones. Subtracting row j from

all other rows yields

$$\mathring{X}_{ij} = (-1)^{i+j}\det \begin{bmatrix} -\lambda-1 & 0 & \cdots & \overset{i\text{-th col}}{0} & \cdots & 0 \\ 0 & -\lambda-1 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & -\lambda-1 \end{bmatrix}$$

The i th column now has only one non zero element at row j, such that the deter minant is equal to $(-1)^{i+j}$ times the minor of element (j,i), which is $(-1)^{m-2}(\lambda+1)^{m-2}$. Hence, the adjoint matrix has all elements equal to $(-1)^{m-2}(\lambda+1)^{m-2}$ ex cept for the diagonal elements that are equal to $(-1)^{m-2}(\lambda+1)^{m-2}(\lambda+2-m)$,

$$\begin{aligned}
\operatorname{adj}(X) &= (-1)^{m-2}(\lambda+1)^{m-2}J \\
&\quad + \left(-(-1)^{m-2}(\lambda+1)^{m-2} + (-1)^{m-2}(\lambda+1)^{m-2}(\lambda+2-m)\right)I \\
&= (-1)^{m-2}(\lambda+1)^{m-2}J + (-1)^{m-2}(\lambda+1)^{m-2}(\lambda+1-m)I \\
&= (-1)^{m-2}(\lambda+1)^{m-2}\left(J + (\lambda+1-m)I\right)
\end{aligned}$$

and, since $\det X = (-1)^{m-1}(\lambda+1)^{m-1}(\lambda+1-m)$, the inverse matrix of X is

$$X^{-1} = -\frac{1}{(\lambda+1)(\lambda+1-m)}\left(J+(\lambda+1-m)I\right)_{m\times m} \tag{5.17}$$

We now compute

$$\begin{aligned}
Y &= J_{(N-m)\times m}X^{-1}_{m\times m}J_{m\times(N-m)} \\
&= -\frac{1}{(\lambda+1)(\lambda+1-m)}J_{(N-m)\times m}\left(J_{m\times m}+(\lambda+1-m)I_{m\times m}\right)J_{m\times(N-m)}
\end{aligned}$$

Using $J_{k\times n}J_{n\times l} = nJ_{k\times l}$ gives

$$\begin{aligned}
Y &= -\frac{1}{(\lambda+1)(\lambda+1-m)}\left(mJ_{(N-m)\times m}+(\lambda+1-m)J_{(N-m)\times m}\right)J_{m\times(N-m)} \\
&= -\frac{1}{(\lambda+1)(\lambda+1-m)}\left(m^2 J_{(N-m)\times(N-m)}+m(\lambda+1-m)J_{(N-m)\times(N-m)}\right)
\end{aligned}$$

whence

$$Y = -\frac{m}{(\lambda+1-m)}J_{(N-m)\times(N-m)} \tag{5.18}$$

Combining all yields

$$\begin{aligned}
\det(A_{m\text{star}}-\lambda I) &= \det\left(J-(\lambda+1)I\right)_{m\times m}\det\left(\frac{m}{\lambda+1-m}J-\lambda I\right)_{(N-m)\times(N-m)} \\
&= \det(X)\left(\frac{m}{\lambda+1-m}\right)^{N-m}\det\left(J-\frac{\lambda(\lambda+1-m)}{m}I\right)
\end{aligned}$$

Finally, using (5.1) leads to

$$\det\left(A_{m\text{star}} - \lambda I\right) = (-1)^N \left(\frac{m}{(\lambda+1-m)}\right)^{N-m} (\lambda+1)^{m-1}(\lambda+1-m)$$

$$\times \left(\frac{\lambda(\lambda+1-m)}{m}\right)^{N-m-1}\left(\frac{\lambda(\lambda+1-m)}{m} - N + m\right)$$

$$= (-1)^N (\lambda+1)^{m-1}\lambda^{N-m-1}\left(\lambda(\lambda+1-m) - m(N-m)\right)$$

$$\tag{5.19}$$

$$= (-1)^N (\lambda+1)^{m-1}\lambda^{N-m-1}(\lambda-\alpha_-)(\lambda-\alpha_+)$$

where

$$\alpha_\pm = \frac{m-1}{2} \pm \sqrt{m(N-m) + \left(\frac{m-1}{2}\right)^2}$$

The eigenvalues of $A_{m\text{star}}$ are α_-, $[-1]^{m-1}$, $[0]^{N-1-m}$, and $(\lambda_{\max})_{m\text{star}} = \alpha_+$, which is larger than $(\lambda_{\max})_{K_{m,n}} = \sqrt{m(N-m)}$ as was expected from Gerschgorin's The orem 36. When viewing the complete spectrum, we observe that (a) the spectrum is not symmetric in λ anymore for $m > 1$ and (b) that all other eigenvalues are very small, except for $\lambda = -|\beta| < \alpha_-$, which is $\beta = O(\alpha_-) = O\left(\sqrt{mN}\right)$.

If $m = N-1$, the $m$star topology equals K_N. It is readily verified that, indeed, for $m = N-1$, the spectrum reduces to that of K_N. If $m = N-2$, then the $m$star topology equals K_N minus one link, for which the eigenvalues are α_-, $[-1]^{N-3}$, 0, and

$$(\lambda_{\max})_{m\text{star}} = \alpha_+ = \frac{N-3}{2}\left\{1 + \sqrt{1 + \frac{8(N-2)}{(N-3)^2}}\right\}$$

$$= N-1 - 2\frac{(N^2-2N-1)}{(N-3)^3} + O\left(N^{-2}\right)$$

Hence, by deleting one link in the complete graph K_N, the spectral gap (**art.** 55) reduces from N to $\alpha_+ < N-1$. The spectral gap of the complete multi partite graph (Section 5.9) equals $N-2$, when $k = 2$ and $N = 2m$. In that case, m links are removed from the complete graph K_N in such a way that each node has still degree $N-2$.

The second, considerably more efficient way of computing $\det\left(A_{m\text{star}} - \lambda I\right)$ is based on (8.80),

$$\det\left(A_{m\text{star}} - \lambda I\right) = (-\lambda)^{N-m}\det\left((J - (\lambda+1)I)_{m\times m} + \frac{1}{\lambda}J_{m\times(N-m)}J_{(N-m)\times m}\right)$$

Using $J_{k\times n}J_{n\times l} = nJ_{k\times l}$ and (5.1) leads, after some manipulations, to (5.19). The first, elaborate computation supplies us with the matrices X^{-1} in (5.17) and Y in (5.18), that will be of use later in Sections 5.10.2 and 5.10.3.

The spectrum of A_{mstar} can be determined in yet another way[3]. Since A_{mstar} has $N - m$ identical rows, it has an eigenvalue 0 with multiplicity at least $N - m - 1$. Further, since $A_{mstar} + I$ has m identical rows, it follows that A_{mstar} has an eigenvalue -1 with multiplicity at least equal to $m - 1$. The remaining two other eigenvalues are obtained after determining the eigenvector that is orthogonal to the eigenvector (with constant components) belonging to $\lambda = 0$ and that belonging to $\lambda = -1$.

5.10.1 Fully-interconnected stars linked to two separate groups

In stead of the $J_{m \times (N-m)}$ matrix in A_{mstar} of Section 5.10, a next step is to consider some matrix B. Thus, instead of connecting each of the m fully interconnected stars to all other non star nodes, each such star does not necessarily need to connect to all other nodes, but to a few.

Let us consider

$$A_{lmnstar} = \begin{bmatrix} A_{m \times m} & B_{m \times (N-m)} \\ B^T_{(N-m) \times m} & O_{(N-m) \times (N-m)} \end{bmatrix}$$

where

$$B = \begin{bmatrix} J_{n \times l} & O_{n \times (N-m-l)} \\ O_{(m-n) \times l} & J_{(m-n) \times (N-m-l)} \end{bmatrix}$$

which means that n stars all reach the same l nodes and $m - n$ stars all reach $N - m - l$ other nodes. The eigenvalue analysis is simplified if we consider $A = O$. Then, using (8.79) gives

$$\det\left(A_{lmnstar} - \lambda I\right) = (-\lambda)^m \det\left(-\lambda I + \frac{1}{\lambda} B^T B\right)$$

where

$$
\begin{aligned}
B^T B &= \begin{bmatrix} J^T_{n \times l} & O^T_{(m-n) \times l} \\ O^T_{n \times (N-m-l)} & J^T_{(m-n) \times (N-m-l)} \end{bmatrix} \begin{bmatrix} J_{n \times l} & O_{n \times (N-m-l)} \\ O_{(m-n) \times l} & J_{(m-n) \times (N-m-l)} \end{bmatrix} \\
&= \begin{bmatrix} J_{l \times n} & O_{l \times (m-n)} \\ O_{(N-m-l) \times n} & J_{(N-m-l) \times (m-n)} \end{bmatrix} \begin{bmatrix} J_{n \times l} & O_{n \times (N-m-l)} \\ O_{(m-n) \times l} & J_{(m-n) \times (N-m-l)} \end{bmatrix} \\
&= \begin{bmatrix} n J_{l \times l} & O_{l \times (N-m-l)} \\ O_{(N-m-l) \times l} & (m-n) J_{(N-m-l) \times (N-m-l)} \end{bmatrix}
\end{aligned}
$$

---

[3] This method was pointed out to me by E. van Dam.

Thus,

$$b = \det\left(-\lambda I + \frac{1}{\lambda}B^T B\right) = \det\left(\frac{1}{\lambda}\left(B^T B - \lambda^2 I\right)\right)$$

$$= \lambda^{-m-N}\det\left(B^T B - \lambda^2 I\right)$$

$$= \lambda^{-m-N}\det\begin{bmatrix} nJ_{l\times l} - \lambda^2 I & O_{l\times(N-m-l)} \\ O_{(N-m-l)\times l} & (m-n)J_{(N-m-l)\times(N-m-l)} - \lambda^2 I \end{bmatrix}$$

$$= \lambda^{-m-N}\det\left(nJ_{l\times l} - \lambda^2 I\right)\det\left((m-n)J_{(N-m-l)\times(N-m-l)} - \lambda^2 I\right)$$

$$= \lambda^{-m-N}n^l\det\left(J_{l\times l} - \frac{\lambda^2}{n}I\right)(m-n)^{N-m-l}$$

$$\times \det\left(J_{(N-m-l)\times(N-m-l)} - \frac{\lambda^2}{m-n}I\right)$$

With (5.1), we arrive at

$$\det\left(A_{lmnstar} - \lambda I\right) = (-\lambda)^m \lambda^{-m-N}n^l(-1)^{l-1}\left(\frac{\lambda^2}{n}\right)^{l-1}\left(\frac{\lambda^2}{n}-l\right)(m-n)^{N-m-l}$$

$$\times (-1)^{N-m-l-1}\left(\frac{\lambda^2}{m-n}\right)^{N-m-l-1}\left(\frac{\lambda^2}{m-n}-N+m+l\right)$$

$$= (-1)^N\lambda^{N-4}\left(\lambda^2 - nl\right)\left(\lambda^2 - (N-m-l)(m-n)\right)$$

and the eigenvalues of $A_{lmnstarG}$ are $\pm\sqrt{nl}, \pm\sqrt{(N-m-l)(m-n)}$ and $[0]^{N-4}$.

For $l = n = 0$, the spectrum reduces to that of $K_{m,N-m}$ (as it should since $A_{lmnstar} = K_{m,N-m}$).

5.10.2 Star-like, two-hierarchical structure

We compute the spectrum of a classical star like, two hierarchical telephony network where

$$A_{mdoublestar} = \begin{bmatrix} (J-I)_{m\times m} & B_{m\times(N-m)} \\ B^T_{(N-m)\times m} & O_{(N-m)\times(N-m)} \end{bmatrix}$$

where

$$B = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 & 0 & \cdots & \cdots & 0 \\ 0 & \cdots & 0 & 1 & \cdots & 1 & 0 & \cdots & \cdots & 0 \\ \vdots & & & & \vdots & & & & & \vdots \\ 0 & \cdots & & & & \cdots & 0 & 1 & \cdots & 1 \end{bmatrix} = I_{m\times m} \otimes u_{1\times l}$$

with $u_{1\times l}$ is the l component long all one vector and the Kronecker product is defined in **art.** 185. Thus, the dimension of B is $m \times lm$ and $N - m = lm$, and the number of nodes in $A_{\text{doublestar}}$ is $N = (l+1)m$. All m fully interconnected nodes $(A_{m\times m} = (J-I)_{m\times m})$ may represent the highest level core in a telephony

network. Each of these m nodes connects to l different lower level nodes, the local exchanges, in the telephony network.

Applying (8.79) and denoting $X_{m\times m} = (J - (\lambda + 1)\,I)_{m\times m}$, the characteristic polynomial is

$$\det\left(A_{m\text{doublestar}} - \lambda I\right) = \det\left(X\right)\det\left(-\lambda I - B^T_{(N-m)\times m}X^{-1}_{m\times m}B_{m\times(N-m)}\right)$$

In Section 5.10, the inverse of $X_{m\times m} = (J - (\lambda + 1)\,I)_{m\times m}$ is computed in (5.17). Thus,

$$B^T_{(N-m)\times m}X^{-1}_{m\times m}B_{m\times(N-m)} = -\frac{B^T_{(N-m)\times m}\left(J + (\lambda + 1 - m)\,I\right)_{m\times m}B_{m\times(N-m)}}{(\lambda + 1)(\lambda + 1 - m)}$$

Further, with

$$J_{m\times m}B_{m\times(N-m)} = J_{m\times m}\left(I_{m\times m}\otimes u_{1\times l}\right) = \left(J_{m\times m}\otimes u_{1\times 1}\right)\left(I_{m\times m}\otimes u_{1\times l}\right)$$
$$= \left(J_{m\times m}I_{m\times m}\otimes u_{1\times 1}u_{1\times l}\right) = J_{m\times m}\otimes u_{1\times l} = J_{m\times ml}$$

and, similarly,

$$B^T_{(N-m)\times m}J_{m\times ml} = \left(I_{m\times m}\otimes u_{l\times 1}\right)\left(J_{m\times m}\otimes u_{1\times l}\right) = J_{m\times m}\otimes u_{l\times 1}u_{1\times l}$$
$$= J_{m\times m}\otimes J_{l\times l} = J_{ml\times ml}$$

we obtain, using properties of the Kronecker product (Meyer, 2000, p. 598), that

$$Y = B^T_{(N-m)\times m}\left(J + (\lambda + 1 - m)\,I\right)_{m\times m}B_{m\times(N-m)}$$
$$= B^T_{(N-m)\times m}J_{m\times ml} + (\lambda + 1 - m)\,B^T_{(N-m)\times m}B_{m\times(N-m)}$$
$$= J_{ml\times ml} + (\lambda + 1 - m)\left(I_{m\times m}\otimes u_{l\times 1}\right)\left(I_{m\times m}\otimes u_{1\times l}\right)$$
$$= J_{ml\times ml} + (\lambda + 1 - m)\left(I_{m\times m}\otimes u_{l\times 1}u_{1\times l}\right)$$
$$= J_{m\times m}\otimes J_{l\times l} + (\lambda + 1 - m)\left(I_{m\times m}\otimes J_{l\times l}\right)$$
$$= \left\{J_{m\times m} + (\lambda + 1 - m)\,I_{m\times m}\right\}\otimes J_{l\times l}$$

Hence,

$$C = \det\left(-\lambda I - B^T_{(N-m)\times m}\left(J - (\lambda + 1)\,I\right)^{-1}_{m\times m}B_{m\times(N-m)}\right)$$
$$= \det\left(-\lambda I + \frac{1}{(\lambda + 1)(\lambda + 1 - m)}\left\{J_{m\times m} + (\lambda + 1 - m)\,I_{m\times m}\right\}\otimes J_{l\times l}\right)$$
$$= \frac{\det\left(-\lambda(\lambda + 1)(\lambda + 1 - m)\,I + \left\{J_{m\times m} + (\lambda + 1 - m)\,I_{m\times m}\right\}\otimes J_{l\times l}\right)}{(\lambda + 1)^{ml}(\lambda + 1 - m)^{ml}}$$

The eigenvalues of $D_{m\times m}\otimes E_{l\times l}$ are the ml numbers $\{\lambda_j(D)\,\lambda_k(E)\}_{1\le j\le m, 1\le k\le l}$ (**art.** 185). The eigenvalues of $D = J_{m\times m} + (\lambda + 1 - m)\,I_{m\times m}$ follow from (5.1) as $\lambda(D) = \left\{[\lambda + 1 - m]^{m-1}, \lambda + 1\right\}$, while the eigenvalues of $E = J_{l\times l}$ are $\lambda(E) = \left\{[0]^{l-1}, l\right\}$. Hence, $\det\left(D_{m\times m}\otimes E_{l\times l} - zI\right) = 0$ has the zeros $[0]^{ml-m}, l(\lambda + 1)$

and $[l(\lambda + 1 - m)]^{m\,1}$ and the same as the polynomial

$$z^{ml\ m}(z - l(\lambda + 1))(z - l(\lambda + 1 - m))^{m\,1}$$

such that the polynomial C in λ has, with $z^* = \lambda(\lambda + 1)(\lambda + 1 - m)$, the same zeros as

$$C^* = \left. \frac{z^{ml\ m}(z - l(\lambda + 1))(z - l(\lambda + 1 - m))^{m\,1}}{(\lambda + 1)^{ml}(\lambda + 1 - m)^{ml}} \right|_{z=z^*}$$

Combined, again using (5.1), yields

$$\det(A_{m\text{doublestar}} - \lambda I) = \alpha(-1)^m (\lambda + 1)^{m\,1}(\lambda + 1 - m)$$
$$\times \left. \frac{z^{ml\ m}(z - l(\lambda + 1))(z - l(\lambda + 1 - m))^{m\,1}}{(\lambda + 1)^{ml}(\lambda + 1 - m)^{ml}} \right|_{z=z^*}$$

Simplified,

$$\det(A_{m\text{doublestar}} - \lambda I) = \alpha(-1)^m \lambda^{ml\ m}(\lambda(\lambda + 1 - m) - l)(\lambda(\lambda + 1) - l)^{m\,1}$$

The eigenvalues of $A_{m\text{doublestar}}$ are, beside a high multiplicity root at zero $[0]^{ml\ m}$, $\frac{m\,1}{2} \pm \frac{1}{2}\sqrt{(m-1)^2 + 4l}$ and $\left[-\frac{1}{2} \pm \frac{1}{2}\sqrt{1 + 4l}\right]^{m\,1}$. The number of different eigen values equals four, which implies that the diameter is three (**art. 39**).

The double star with $m = 2$ and $N = 2(l + 1)$ is proved in Das and Kumar (2004) to have as largest eigenvalue

$$\lambda_{\max}(A_{2\text{doublestar}}) = \sqrt{\frac{(N-1) + \sqrt{2N - 3}}{2}} = \frac{1}{2} + \frac{1}{2}\sqrt{2N - 3}$$

5.10.3 Complementary double cone

We consider a complete graph K_N to which two nodes, labeled by $N+1$ and $N+2$, are connected. Node $N + 1$ is connected to m nodes in K_N and node $N + 2$ to the $N - m$ other nodes. The corresponding adjacency matrix of this complementary double cone (CDC) on K_N is

$$A_{CDC} = \begin{bmatrix} (J - I)_{N \times N} & B_{N \times 2} \\ B_{2 \times N}^T & O_{2 \times 2} \end{bmatrix}_{(N+2) \times (N+2)}$$

where

$$B_{N \times 2} = \begin{bmatrix} u_{m \times 1} & 0_{m \times 1} \\ 0_{(N\ m) \times 1} & u_{(N\ m) \times 1} \end{bmatrix}$$

The CDC graph has diameter 3 and each other graph with diameter 3 is a subgraph of CDC (see also **art.** 42 on strongly regular graphs). The corresponding Laplacian is

$$Q_{CDC} = \begin{bmatrix} NI - (J - I)_{N \times N} & -B_{N \times 2} \\ -B_{2 \times N}^T & \text{diag}(m, N - m) \end{bmatrix}$$

whose eigenvalues follow from

$$\det\left(Q_{CDC} - \mu I\right) = \det\begin{bmatrix} (N+1-\mu)I - J_{N\times N} & -B_{N\times 2} \\ -B^T_{2\times N} & \operatorname{diag}(m-\mu, N-m-\mu) \end{bmatrix}$$

We apply (8.80), with $D = \operatorname{diag}(m-\mu, N-m-\mu)$, whose inverse is $D^{-1} = \operatorname{diag}\left((m-\mu)^{-1}, (N-m-\mu)^{-1}\right)$, and

$$BD^{-1}C = B_{N\times 2}\operatorname{diag}\left((m-\mu)^{-1}, (N-m-\mu)^{-1}\right)B^T_{2\times N}$$

$$= \begin{bmatrix} u_{m\times 1} & 0_{m\times 1} \\ 0_{(N-m)\times 1} & u_{(N-m)\times 1} \end{bmatrix}\begin{bmatrix} \frac{1}{m-\mu} & 0 \\ 0 & \frac{1}{N-m-\mu} \end{bmatrix}\begin{bmatrix} u_{1\times m} & 0_{1\times(N-m)} \\ 0_{1\times m} & u_{1\times(N-m)} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{m-\mu}J_{m\times m} & O_{m\times(N-m)} \\ O_{(N-m)\times m} & \frac{1}{N-m-\mu}J_{(N-m)\times(N-m)} \end{bmatrix}$$

such that, with $A = (N+1-\mu)I - J_{N\times N}$, we obtain

$$T = A - BD^{-1}C$$

$$= \begin{bmatrix} (N+1-\mu)I_{m\times m} - \left(\frac{1}{m-\mu}+1\right)J & -J_{m\times(N-m)} \\ -J_{(N-m)\times m} & (N+1-\mu)I - \left(\frac{1}{N-m-\mu}+1\right)J \end{bmatrix}$$

Hence,

$$\det\left(Q_{CDC} - \mu I\right) = \det D \det T$$

$$= (m-\mu)(N-m-\mu)\det T$$

The determinant of T is computed with (8.79). The computation is similar to those of m fully connected stars in Section 5.10. Using (5.16), we express the matrix as

$$(N+1-\mu)I_{m\times m} - \frac{1+m-\mu}{m-\mu}J_{m\times m} = -\frac{1+m-\mu}{m-\mu}X_{m\times m}$$

where $\lambda + 1 = \frac{m-\mu}{1+m-\mu}(N+1-\mu)$. With (5.18), we have

$$-\frac{m-\mu}{1+m-\mu}J_{(N-m)\times m}X^{-1}J_{m\times(N-m)} = \frac{(m-\mu)}{(1+m-\mu)}\frac{m}{(\lambda+1-m)}J_{(N-m)\times(N-m)}$$

such that, with $\theta = \frac{(m-\mu)}{(1+m-\mu)}\frac{m}{(\lambda+1-m)} + \frac{N-m-\mu+1}{N-m-\mu}$,

$$\det T = \det\left(-\frac{1+m-\mu}{m-\mu}X_{m\times m}\right)\det\left((N+1-\mu)I_{(N-m)\times(N-m)} - \theta J\right)$$

$$= \left(-\frac{1+m-\mu}{m-\mu}\right)^m (-\theta)^{N-m}\det\left((J-(\lambda+1)I)_{m\times m}\right)$$

$$\times \det\left(J - \frac{N+1-\mu}{\theta}I\right)$$

Using (5.1) yields

$$\det T = \left(\frac{1+m-\mu}{m-\mu}\right)(\lambda+1-m)(N+1-\mu)^{N-2}(N+1-\mu-(N-m)\theta)$$

After simplification, we find that

$$\theta = \frac{m(N-m)(N+1)-\mu\{(N+1)^2-m+m(N-m)\}+2(N+1)\mu^2-\mu^3}{(m(N-m)-\mu(N+1)+\mu^2)(N-m-\mu)}$$

We now compute $N+1-\mu-(N-m)\theta = \frac{s(\mu)}{r}$, where

$$r = \left(m(N-m)-\mu(N+1)+\mu^2\right)(N-m-\mu)$$

The result is

$$s(\mu) = \mu\left(\mu^3-2\mu^2(N+1)+\mu\{(N+1)^2+m(N-m)\}-m(N-m)(N+2)\right)$$

The polynomial $\frac{s(\mu)}{\mu}$ has degree 3 in μ and the sum of its zeros is $2(N+1)$, while the product is $m(N-m)(N+2)$.

Combining all factors yields

$$\det T = \frac{1}{(m-\mu)(N-m-\mu)}(N+1-\mu)^{N-2}s(\mu)$$

and

$$\det(Q_{CDC}-\mu I) = \det D \det T$$
$$= (N+1-\mu)^{N-2}s(\mu)$$

In summary, the eigenvalues of $(Q_{CDC})_{(N+2)\times(N+2)}$ are 0, $[N+1]^{N-2}$, and the three real positive roots of $s(\mu)$.

5.11 A chain of cliques

A chain of $D+1$ cliques is a graph $G_D^*(n_1, n_2, ..., n_{D+1})$ consisting of $D+1$ complete graphs K_{n_j} (clique) with $1 \le j \le D+1$ where each clique K_{n_j} is fully interconnected with its neighboring cliques $K_{n_{j-1}}$ and $K_{n_{j+1}}$. Two graphs G_1 and G_2 are fully interconnected if each node in G_1 is connected to each node in G_2. An example of a member of the class $G_D^*(n_1, n_2, ..., n_{D+1})$ is drawn in Fig. 5.5. The total number of nodes in $G_D^*(n_1, n_2, ..., n_{D+1})$ is

$$N = \sum_{j=1}^{D+1} n_j \tag{5.20}$$

The total number of links in G_D^* is

$$L = \sum_{j=1}^{D+1}\binom{n_j}{2} + \sum_{j=1}^{D} n_j n_{j+1} \tag{5.21}$$
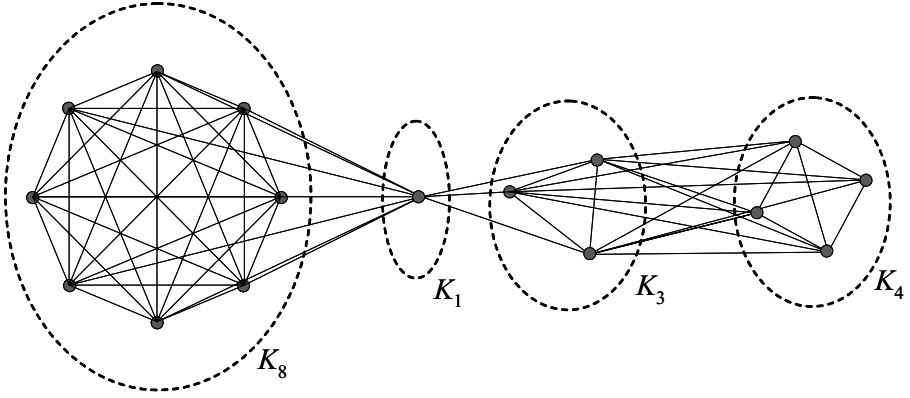
Fig. 5.5. A chain of cliques $G_4^*(8, 1, 3, 4)$.

where the first sum equals the number of intra cluster links and the second the number of inter cluster links. The main motivation to study the class of graphs $G_D^*(n_1, n_2, ..., n_{D+1})$ with $n_j \geq 1$ are its extremal properties, which are proved in Wang *et al.* (2010b):

Theorem 23 *Any graph $G(N, D)$ with N nodes and diameter D is a subgraph of at least one graph in the class $G_D^*(n_1 = 1, n_2, ..., n_D, n_{D+1} = 1)$.*

Theorem 24 *The maximum of any Laplacian eigenvalue $\mu_i(G_D^*)$, $i \in [1, N]$ achieved in the class $G_D^*(n_1 = 1, n_2, ..., n_D, n_{D+1} = 1)$ is also the maximum among all the graphs with N nodes and diameter D.*

Theorem 25 *The maximum number of links in a graph with given size N and diameter D is $L_{\max}(N, D) = \binom{N \quad D+2}{2} + D - 3$, which can only be obtained by either $G_D^*(1, ..., 1, n_j = N - D, 1, ..., 1)$ with $j \in [2, D]$, where only one clique has size larger than one, or by $G_D^*(1, ..., 1, n_j > 1, n_{j+1} > 1, 1, ..., 1)$ with $j \in [2, D-1]$ where only two cliques have size larger than one and they are next to each other.*

Another valuable theorem, due to van Dam (2007) and related to Theorem 25, is:

Theorem 26 *The graph $G_D^*(n_1, n_2, ..., n_{D+1})$ with $n_{\left[\frac{D+1}{2}\right]} = N - D$ and all other $n_j = 1$ is the graph with largest spectral radius (i.e., the largest eigenvalue of the adjacency matrix) among all graphs with a same diameter D and number of nodes N.*

Here, we will compute the Laplacian spectrum of $G_D^*(n_1, n_2, ..., n_{D-1}, n_D, n_{D+1})$: we will show that $N - D$ eigenvalues are exactly known, while the remain D eigen values are the positive zeros of an orthogonal polynomial. The adjacency matrix

$A_{G_D^*}$ of $G_D^*(n_1, n_2, ..., n_{D\ 1}, n_D, n_{D+1})$ is

$$
\begin{bmatrix}
\widetilde{J}_{n_1 \times n_1} & J_{n_1 \times n_2} \\
J_{n_2 \times n_1} & \widetilde{J}_{n_2 \times n_2} & J_{n_2 \times n_3} \\
& & \ddots \\
& & J_{n_i \times n_i\ 1} & \widetilde{J}_{n_i \times n_i} & J_{n_i \times n_{i+1}} \\
& & & & \ddots \\
& & & & J_{n_{D+1} \times n_{D+1}} & \widetilde{J}_{n_{D+1} \times n_{D+1}}
\end{bmatrix}
$$

where $\widetilde{J} = J - I$.

Theorem 27 *The characteristic polynomial of the Laplacian $Q_{G_D^*}$ of the class of graphs $G_D^*(n_1, n_2, ..., n_{D+1})$ equals*

$$
\det\left(Q_{G_D^*} - \mu I\right) = p_D(\mu) \prod_{j=1}^{D+1} (d_j + 1 - \mu)^{n_j\ 1} \tag{5.22}
$$

where $d_j = n_{j\ 1} + n_j + n_{j+1} - 1$ denotes the degree of a node in clique j. The polynomial $p_D(\mu) = \prod_{j=1}^{D+1} \theta_j$ is of degree $D+1$ in μ and the function $\theta_j = \theta_j(D; \mu)$ obeys the recursion

$$
\theta_j = (d_j + 1 - \mu) - \left(\frac{n_{j\ 1}}{\theta_{j\ 1}} + 1\right) n_j \tag{5.23}
$$

with initial condition $\theta_0 = 1$ and with the convention that $n_0 = n_{D+2} = 0$.

The proof below elegantly uses the concept of a quotient matrix, defined in Section 2.1.3. An elementary, though more elaborated proof, which is basically an extension of the derivation in Section 5.10.3, is found in Van Mieghem and Wang (2009). Consider the k partition of a graph G that separate the node set $\mathcal{N}$ of G into $k \in [1, N]$ disjoint, non empty subsets $\{\mathcal{N}_1, \mathcal{N}_2, ..., \mathcal{N}_k\}$. Correspondingly, the quotient matrix A^π of the adjacency matrix of G is a $k \times k$ matrix, where $A_{i,j}^\pi$ is the average number of neighbors in $\mathcal{N}_j$ of nodes in $\mathcal{N}_i$. Similarly, the quotient matrix Q^π of the Laplacian matrix Q of G is a $k \times k$ matrix, where

$$
Q_{i,j}^\pi = \begin{cases} -A_{i,j}^\pi, & \text{if } i \neq j \\ \sum_{i \neq k} A_{i,k}^\pi, & \text{if } i = j \end{cases}
$$

As defined in **art. 15**, a partition is called regular or equitable if for all $1 \leq i, j \leq k$ the number of neighbors in $\mathcal{N}_j$ is the same for all the nodes in $\mathcal{N}_i$. The eigenvalues derived from the quotient matrix A^π (Q^π) of the adjacency A (Laplacian Q) matrix are also eigenvalues of A (Laplacian Q) given the partition is equitable (see **art. 15**).

Proof: The partition that separates the graph $G_D^*(n_1, n_2, ..., n_{D+1})$ into the $D + 1$ cliques $K_{n_1}, K_{n_2}, ..., K_{n_{D+1}}$ is equitable. The quotient matrix Q^π of the

Laplacian matrix Q of G is

$$
Q^{\pi} = \begin{bmatrix}
n_2 & -n_2 & & & & & \\
-n_1 & n_1 + n_3 & -n_3 & & & & \\
& -n_2 & n_2 + n_4 & -n_4 & & & \\
& & & \ddots & & & \\
& & & & -n_{D\ 1} & n_{D\ 1} + n_{D+1} & -n_{D+1} \\
& & & & & -n_D & n_D
\end{bmatrix}
$$

$$(5.24)$$

We use (8.79) to $\det (Q^{\pi} - \mu I)$

$$
= \begin{vmatrix}
n_2 - \mu & -n_2 & & & & & \\
-n_1 & n_1 + n_3 - \mu & -n_3 & & & & \\
& -n_2 & n_2 + n_4 - \mu & -n_4 & & & \\
& & & \ddots & & & \\
& & & & -n_{D\ 1} & n_{D\ 1} + n_{D+1} - \mu & -n_{D+1} \\
& & & & & -n_D & n_D - \mu
\end{vmatrix}
$$

$$
= (n_2 - \mu) \begin{vmatrix}
n_1 + n_3 - \mu - \frac{n_1 n_2}{n_2\ \mu} & -n_3 & & \\
-n_2 & n_2 + n_4 - \mu & -n_4 & \\
& & \ddots & \\
& & & n_D - \mu
\end{vmatrix}
$$

We repeat the method and obtain

$$
\det (Q^{\pi} - \mu I) = (n_2 - \mu) \left(n_1 + n_3 - \mu - \frac{n_1 n_2}{n_2 - \mu} \right) \times
$$

$$
\det \begin{bmatrix}
n_2 + n_4 - \mu - \frac{n_2 n_3}{\left(n_1 + n_3\ \mu\ \frac{n_1 n_2}{n_2\ \mu} \right)} & -n_4 & & & \\
& \ddots & & & \\
& & -n_{D\ 1} & n_{D\ 1} + n_{D+1} - \mu & -n_{D+1} \\
& & & -n_D & n_D - \mu
\end{bmatrix}
$$

Eventually, after subsequent expansions using (8.79), we find

$$
\det (Q^{\pi} - \mu I) = \prod_{j=1}^{D+1} \theta_j = p_D (\mu)
$$

where θ_j follows the recursion

$$
\theta_j = (n_{j\ 1} + n_{j+1} - \lambda) - \frac{n_{j\ 1} n_j}{\theta_{j\ 1}}
$$

with initial condition $\theta_0 = 1$ and with the convention that $n_0 = n_{D+2} = 0$. When written in terms of the degree $d_j = n_{j\ 1} + n_j + n_{j+1} - 1$, we obtain (5.23).

Any two nodes s and t in a same clique K_{n_i} of G_D^* are connected to each other and they are connected to the same set of neighbors. The two rows in $\det \left(Q_{G_D^*} - \mu I \right)$

corresponding to node s and t are the same when $\mu = d_i + 1$, where d_i is the degree of all nodes in clique K_{n_i}. In this case, $\det \left(Q_{G_D^*} - \mu I \right) = 0$ since the rank of $Q_{G_D^*} - \mu I$ is reduced by 1. Hence, $\mu = d_i + 1$ is an eigenvalue of the Laplacian matrix $Q_{G_D^*}$. The corresponding eigenvector x has only two non zero components, $x_s = -x_t \neq 0$. Since the $D + 1$ partitions of $G_D^*(n_1, n_2, ..., n_{D+1})$ are equitable, the $D + 1$ eigenvalues of Q^π, which are the roots of $\det (Q^\pi - \mu I) = 0$, are also the eigenvalues of the Laplacian matrix $Q_{G_D^*}$. Each eigenvector of $Q_{G_D^*}$, belonging to the $D + 1$ eigenvalues, has the same elements $x_s = x_t$ if the nodes s and t belong to the same clique. Hence, the Laplacian matrix $Q_{G_D^*}$ has $D + 1$ non trivial eigenvalues, which are the roots of $\det (Q^\pi - \mu I) = 0$ and trivial eigenvalues $d_j + 1$ with multiplicity $n_j - 1$ for $1 \leq j \leq D + 1$. $\qquad \square$

5.11.1 Orthogonal polynomials

In the sequel, we will show that the polynomial $p_D (\mu)$ in Theorem 27 belongs to a set of orthogonal polynomials (see Chapter 10). The dependence of θ_j on the diameter D and on μ is further on explicitly written.

Lemma 4 *For all $j \geq 0$, the functions $\theta_j (D; x)$ are rational functions*

$$\theta_j (D; x) = \frac{t_j (D; x)}{t_{j-1} (D; x)} \tag{5.25}$$

where $t_j (x)$ is a polynomial of degree j in $x = -\mu$ and $t_0 (D; x) = 1$.

Proof: It holds for $j = 1$ as verified from (5.23) because $\theta_0 (D; x) = 1$. Let us assume that (5.23) holds for $j - 1$ (induction argument). Substitution of (5.25) into the right hand side of (5.23),

$$\theta_j (D; x) = \begin{cases} \frac{(x + n_{j-1} + n_{j+1}) t_{j-1} (D;x) \; n_{j-1} n_j t_{j-2} (D;x)}{t_{j-1} (D;x)} & 1 \leq j \leq D \\ \frac{(x + n_D) t_D (D;x) \; n_D n_{D+1} t_{D-1} (D;x)}{t_D (D;x)} & j = D + 1 \end{cases}$$

indeed shows that the left hand side is of the form (5.25) for j. This demonstrates the induction argument and proves the lemma. $\qquad \square$

The polynomial of interest,

$$p_D (\mu) = \prod_{j=1}^{D+1} \theta_j (D; \mu) = \sum_{k=0}^{D+1} c_k (D) \mu^k = \prod_{k=1}^{D+1} (z_k - \mu) \tag{5.26}$$

(where the product with the zeros $z_{D+1} \leq z_D \leq \cdots \leq z_1$ follows from the definition of the eigenvalue equation (8.5)) equals with (5.25)

$$p_D (-x) = \frac{\prod_{j=1}^{D+1} t_j (D; x)}{\prod_{j=1}^{D+1} t_{j-1} (D; x)} = t_{D+1} (D; x)$$

We rewrite (5.25) as $t_j(D;x) = \theta_j(D;x) t_{j-1}(D;x)$ and with (5.23), we obtain the set of polynomials

$$
\begin{cases}
t_{D+1}(D;x) = (x + n_D) t_D(D;x) - n_D n_{D+1} t_{D-1}(D;x) \\
t_j(D;x) = (x + n_{j-1} + n_{j+1}) t_{j-1}(D;x) - n_{j-1} n_j t_{j-2}(D;x) & \text{for } 1 \le j \le D \\
t_1(D;x) = (x + n_2) t_0(D;x)
\end{cases}
$$
(5.27)

where $t_0(D;x) = 1$. **Art.** 248 demonstrates that, for a fixed D, the sequence $\{t_j(D;x)\}_{0 \le j \le D+1}$ is a set of orthogonal polynomials because (5.27) obeys Favard's three term recurrence relation. By Theorem 66, the zeros of any set of orthogonal polynomials are all simple, real and lie in the orthogonality interval $[a, b]$, which is here for the Laplacian equal to $[0, N]$.

By iterating the equation upwards, we find that

$$
t_j(D;0) = \begin{cases}
\displaystyle\prod_{m=2}^{j+1} n_m & 1 \le j \le D \\
0 & j = D+1
\end{cases}
$$
(5.28)

Thus, $t_{D+1}(D;0) = 0$ (and thus $\theta_{D+1}(D;0) = 0$) implies that $p_D(\mu)$ must have a zero at $\mu = 0$, which is, indeed, a general property of any Laplacian (**art.** 66). From (5.25), it then follows that

$$
\theta_j(D;0) = n_{j+1} > 0
$$

The eigenvalues of the Jacobi matrix (**art.** 260),

$$
M = \begin{bmatrix}
-n_2 & 1 & & & & \\
n_1 n_2 & -(n_1 + n_3) & 1 & & & \\
& \ddots & \ddots & & \ddots & \\
& & n_{D-1} n_D & -(n_{D-1} + n_{D+1}) & 1 \\
& & & n_D n_{D+1} & -n_D
\end{bmatrix}
$$
(5.29)

are equal to the zeros of $p_D(-x)$. Moreover, we observe that also the quotient matrix Q^π in (5.24) possesses the same eigenvalues as the Jacobi matrix M. Since the eigenvalues of M are simple, **art.** 142 shows that there exists a similarity transform that maps the Jacobi matrix M into the quotient matrix Q^π (and vice versa). Moreover, the matrix M can be symmetrized by a similarity transform,

$$
H = \operatorname{diag}\left(1, \frac{1}{\sqrt{n_1 n_2}}, \ldots, \frac{1}{\sqrt{n_1 n_j} \displaystyle\prod_{k=2}^{j-1} n_k}, \ldots, \frac{1}{\sqrt{n_1 n_{D+1}} \displaystyle\prod_{k=2}^{D} n_k} \right)
$$

and the eigenvector belonging to zero equals

$$
\tilde{\tau}(D;0) = H\tau(D;0) = \begin{bmatrix} 1 & \sqrt{\frac{n_2}{n_1}} & \cdots & \sqrt{\frac{n_{D-1}}{n_1}} & \sqrt{\frac{n_D}{n_1}} \end{bmatrix}^T
$$

After the similarity transform H, the result is $\widetilde{M} = HMH^{-1}$,

$$
\widetilde{M} = \begin{bmatrix}
-n_2 & \sqrt{n_1 n_2} & & & \\
\sqrt{n_1 n_2} & -(n_1 + n_3) & \sqrt{n_2 n_3} & & \\
& \ddots & \ddots & \ddots & \\
& & \sqrt{n_{D-1} n_D} & -(n_{D-1} + n_{D+1}) & \sqrt{n_D n_{D+1}} \\
& & & \sqrt{n_D n_{D+1}} & -n_D
\end{bmatrix}
$$

The corresponding square root matrix A of the Gram matrix $-M = A^T A$ can be computed explicitly as

$$
A = \begin{bmatrix}
\sqrt{n_2} & -\sqrt{n_1} & & \\
0 & \sqrt{n_3} & -\sqrt{n_2} & \\
& \ddots & \ddots & \ddots \\
& & 0 & \sqrt{n_{D+1}} & -\sqrt{n_D} \\
& & & 0 & 0
\end{bmatrix}
$$

in contrast to the general theory in **art. 264**, where each element is a continued fraction.

In summary, all non trivial eigenvalues of $Q_{G_D^*}$ are also eigenvalues of the simpler matrices Q^π, $-M$ or $-\widetilde{M}$. Properties and bounds on those nontrivial eigenvalues and zeros of $p_D(\mu)$ as well as the spectrum of the corresponding adjacency matrix are studied in Van Mieghem and Wang (2009). We mention the asymptotic scaling law:

Theorem 28 *For a constant diameter D and a large number N of nodes, all non trivial eigenvalues of both the adjacency and Laplacian matrix of any graph in the class $G_D^*(n_1, n_2, ..., n_{D+1})$ scale linearly with N, the number of nodes.*

All coefficients $c_k(D)$ of $p_D(\mu)$ in (5.26) can be computed explicitly in terms of the clique sizes $n_1, n_2, \ldots, n_{D+1}$ for which we refer to Van Mieghem and Wang (2009). We merely list here the first few polynomials $q_D(\mu) = \frac{p_D(\mu)}{\mu}$:

$q_1(\mu)$ $(\mu - N)$

$q_2(\mu)$ $\mu^2 - (N + n_2)\mu + Nn_2$ $(\mu - N)(\mu - n_2)$

$q_3(\mu)$ $\mu^3 + (2N - n_1 - n_4)\mu^2 - (n_2^2 + n_3^2 + n_1 n_2 + n_1 n_3 + n_1 n_4 + 3n_2 n_3 + n_2 n_4 + n_3 n_4)\mu$
     $+ Nn_2 n_3$

$q_4(\mu)$ $\mu^4 - (2N - n_1 - n_5)\mu^3$
     $+ (n_2^2 + n_3^2 + n_4^2 + n_4 n_5 + n_3(3n_4 + n_5) + n_2(3n_3 + 3n_4 + 2n_5) + n_1(n_2 + n_3 + 2n_4 + n_5))\mu^2$
     $- (n_3 n_4 (n_3 + n_4 + n_5) + n_2 \{n_3^2 + n_4^2 + 4n_3 n_4 + (n_3 + n_4) n_5 + n_2 (n_3 + n_4 + n_5)\}$
     $+ n_1 (n_2 + n_4)(n_3 + n_4 + n_5))\mu + Nn_2 n_3 n_4$

For increasing D, the explicit expressions rapidly become involved without a simple structure. There is one exception: $G_D^*(n_1, n_2, ..., n_{D+1})$ with all unit size cliques, $n_j = 1$, is a D hop line topology, whose spectrum is exactly given in (5.9), such

that

$$q_D \left(\mu; \{n_j = 1\}_{1 \leq j \leq D+1} \right) = \prod_{k=1}^{D} \left(2 \left(1 - \cos \left(\frac{k\pi}{D+1} \right) \right) - \mu \right)$$

Finally, we mention that $q_3 (\mu)$ appears as the polynomial $s (\mu)$ in the Laplacian spectrum of the complementary double cone (CDC) in Section 5.10.3. The CDC, written as $G_3^* (1, m, N - m, 1)$, is clearly a member of the class $G_D^*(n_1, n_2, ..., n_{D+1})$ with $\sum_{j=1}^{4} n_j = N + 2$.

5.12 The lattice

Consider a rectangular lattice with size z_1 and z_2 where at each lattice point with two integer coordinates (k, l) a node is placed. A node at (k, l) is connected to its direct neighbors at $(k + 1, l)$, $(k - 1, l)$, $(k, l + 1)$ and $(k, l - 1)$ where possible. At border points, nodes only have three neighbors and at the four corner points only two. The number of lattice points (nodes) equals $N = (z_1 + 1)(z_2 + 1)$ and the number of links is $L = 2z_1 z_2 + (z_1 + z_2)$. Meyer (2000) nicely relates the Laplacian of the lattice $G_{\text{La}(N)}$ to the discrete version of the Laplacian operator,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

In a similar vein, Cvetković *et al.* (2009, Chapter 9) discuss the Laplacian operator and its discretization in the solution of the wave equation with rectangular boundary.

The adjacency matrix, following Meyer (2000), is

$$A_{\text{La}(N)} = \begin{bmatrix} T_{(z_1+1) \times (z_1+1)} & I_{(z_1+1) \times (z_1+1)} & & & & \\ I_{(z_1+1) \times (z_1+1)} & T_{(z_1+1) \times (z_1+1)} & I & & & \\ & I_{(z_1+1) \times (z_1+1)} & \ddots & & \ddots & \\ & & \ddots & \ddots & T_{(z_1+1) \times (z_1+1)} & I_{(z_1+1) \times (z_1+1)} \\ & & & & I_{(z_1+1) \times (z_1+1)} & T_{(z_1+1) \times (z_1+1)} \end{bmatrix}$$

where the Toeplitz matrix

$$T_{(z_1+1) \times (z_1+1)} = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 0 & 1 \\ & & & 1 & 0 \end{bmatrix}$$

is the adjacency matrix of a z_1 hops path whose eigenvalues are given by (5.8) with $N \to z_1 + 1$. The Laplacian $Q_{\text{La}(N)}$ is not easily given in general form because the sum of the rows in $A_{\text{La}(N)}$ or the degree of a node is not constant. The adjacency

matrix $A_{\mathrm{La}(N)}$ is a block Toeplitz matrix whose structure is most elegantly written in terms of a Kronecker product. We may verify that[4]

$$A_{\mathrm{La}(N)} = I_{(z_2+1)\times(z_2+1)} \otimes T_{(z_1+1)\times(z_1+1)} + T_{(z_2+1)\times(z_2+1)} \otimes I_{(z_1+1)\times(z_1+1)} \quad (5.30)$$

The eigenvalues of $A_{\mathrm{La}(N)}$ are immediate from **art. 185**. Thus, for all $1 \leq j \leq z_1 + 1, 1 \leq k \leq z_2 + 1$,

$$\lambda_{jk}\left(A_{\mathrm{La}(N)}\right) = \lambda_j\left(T_{(z_1+1)\times(z_1+1)}\right) + \lambda_k\left(T_{(z_2+1)\times(z_2+1)}\right)$$

and with (5.8), we arrive at

$$\lambda_{jk}\left(A_{\mathrm{La}(N)}\right) = 2\cos\left(\frac{\pi j}{z_1+2}\right) + 2\cos\left(\frac{\pi k}{z_2+2}\right)$$

where $1 \leq j \leq z_1 + 1, 1 \leq k \leq z_2 + 1$.

Several extensions are possible. For a cubic or three dimensional lattice, the adjacency matrix generalizes to

$$\begin{aligned}
A_{\mathrm{La}(N)} = {} & I_{(z_3+1)\times(z_3+1)} \otimes I_{(z_2+1)\times(z_2+1)} \otimes T_{(z_1+1)\times(z_1+1)} \\
& + I_{(z_3+1)\times(z_3+1)} \otimes T_{(z_2+1)\times(z_2+1)} \otimes I_{(z_1+1)\times(z_1+1)} \\
& + T_{(z_3+1)\times(z_3+1)} \otimes I_{(z_2+1)\times(z_2+1)} \otimes I_{(z_1+1)\times(z_1+1)}
\end{aligned}$$

with spectrum

$$\lambda_{jkl}\left(A_{\mathrm{La}(N)}\right) = 2\cos\left(\frac{\pi j}{z_1+2}\right) + 2\cos\left(\frac{\pi k}{z_2+2}\right) + 2\cos\left(\frac{\pi l}{z_3+2}\right)$$

where $1 \leq j \leq z_1 + 1, 1 \leq k \leq z_2 + 1, 1 \leq l \leq z_3 + 1$. The Kronecker product where the Toeplitz matrix T of the path is changed for the circulant Toeplitz matrix of the circuit represents a lattice on a torus (Cvetković *et al.*, 1995, p. 74).

We end this section by considering the m dimensional lattice La_m with lengths $z_1, z_2, \ldots, z_m$ in each dimension, respectively, and where at each lattice point with integer coordinates a node is placed that is connected to its nearest neighbors whose coordinates only differ by one in only one components. The total number of nodes in La_m is $N = (z_1 + 1) \times (z_2 + 1) \times \ldots \times (z_m + 1)$. The lattice graph can be written as a Cartesian product (Cvetković *et al.*, 1995) of m path graphs, which we denote

---

[4] When applying the identity (Meyer, 2000, p. 597)

$$(A_1 \otimes B_1)(A_2 \otimes B_2) \quad (A_1 A_2 \otimes B_1 B_2)$$

to compute the square of $A_{\mathrm{La}(N)}^2$ given by (5.30), powers of the Toeplitz matrix appear. However,

$$T_{(z_1+1)\times(z_1+1)}^2 \quad \begin{bmatrix} 1 & 0 & 1 & & & \\ 0 & 2 & 0 & \ddots & & \\ 1 & 0 & \ddots & \ddots & 1 & \\ & \ddots & \ddots & 2 & 0 \\ & & 1 & 0 & 1 \end{bmatrix}$$

shows that the Toeplitz structure is destroyed.

by $\text{La}_m = P_{(z_1+1)} \square P_{(z_2+1)} \square \ldots \square P_{(z_m+1)}$. According to Cvetković *et al.* (1995), the eigenvalues of La_m can be written as a sum of one combination of eigenvalues of path graphs and the corresponding eigenvector is the Kronecker product of the corresponding eigenvectors of the same path graphs,

$$
\begin{aligned}
\lambda_{i_1 i_2 \ldots i_N} (\text{La}_m) &= \textstyle\sum_{j=1}^{m} \lambda_{i_j} \left(P_{(z_j+1)} \right) \\
x_{i_1 i_2 \ldots i_m} (\text{La}_m) &= x_{i_1} \left(P_{(z_j+1)} \right) \otimes x_{i_2} \left(P_{(z_2+1)} \right) \otimes \ldots \otimes x_{i_m} \left(P_{(z_m+1)} \right)
\end{aligned}
\tag{5.31}
$$

where $i_j \in \{1, 2, \ldots, z_j + 1\}$ for each $j \in \{1, 2, \ldots, m\}$. Since both the adjacency and the Laplacian spectrum of the path P_N graph are completely known (Section 5.4), the corresponding spectra of the m dimensional lattice La_m can also analyt ically be computed from (5.31) by substituting $N = z_j + 1$ in the derivations in Section 5.4.

Lemma 5 *The number L of links in the m dimensional lattice La_m is, for $m \geq 1$,*

$$
L = \prod_{j=1}^{m} (z_j + 1) \sum_{j=1}^{m} \frac{z_j}{z_j + 1}
$$

Proof: We will prove the lemma by induction. Let the number of links in the k dimensional lattice La_k be $l(z_1, z_2, \ldots, z_k)$. For $k = 1$, we have a path graph P_{z_1+1} and its number of links is $L = l(z_1) = z_1 = (z_1 + 1)\frac{z_1}{z_1+1}$. Let us assume that the lemma holds for k dimensional lattices. We consider the $(k+1)$ dimensional lattice La_{k+1}, that is constructed from k different k dimensional lattices

$$
\text{La}_{(z_{i_1}+1) \times (z_{i_2}+1) \times \ldots \times (z_{i_k}+1)}, \text{ where } i_1, i_2, \ldots, i_k \in \{1, 2, \ldots, (k+1)\}
$$

in the following way. We position a total of $\left(z_{i_{k+1}} + 1 \right)$ such k dimensional lattices $\text{La}_{(z_{i_1}+1) \times (z_{i_2}+1) \times \ldots \times (z_{i_k}+1)}$ next to each other in the direction of dimension i_{k+1}. In this way, every link is counted k times in each dimensions. Intuitively, this construction is easier to imagine in three dimensions, where the three dimensional lattice $\text{La}_{(z_1+1) \times (z_2+1) \times (z_3+1)}$ is constructed by (z_3+1) consecutive two dimensional $\text{La}_{(z_1+1) \times (z_2+1)}$ planes that are positioned next to each other in the direction of the third dimension, $(z_2 + 1)$ consecutive two dimensional $\text{La}_{(z_1+1) \times (z_3+1)}$ planes that are positioned next to each other in the direction of the second dimension and, finally, $(z_1 + 1)$ consecutive two dimensional La $L_{(z_2+1) \times (z_3+1)}$ planes that are positioned next to each other in the direction of the first dimension. All links in this process are counted twice. Returning to the k dimensional case, we thus deduce that

$$
l(z_1, z_2, \ldots, z_{k+1}) = \frac{1}{k} \sum_{i=1}^{k+1} (z_i + 1) l(z_{j_1}, z_{j_2}, \ldots, z_{j_k})
$$

where $j_w \neq i$ for each $i = 1, 2, \ldots, k+1$ and $w = 1, 2, \ldots, k$. Introducing the

induction hypothesis for k dimensional lattices, we obtain

$$l(z_1, z_2, \ldots, z_{k+1}) = \frac{1}{k} \sum_{i=1}^{k+1} (z_i + 1) \prod_{j=1, j \neq i}^{k+1} (z_j + 1) \sum_{j=1, j \neq i}^{k+1} \frac{z_j}{z_j + 1}$$

$$= \frac{1}{k} \prod_{j=1}^{k+1} (z_j + 1) \sum_{i=1}^{k+1} \sum_{j=1, j \neq i}^{k+1} \frac{z_j}{z_j + 1}$$

$$= \frac{1}{k} \prod_{j=1}^{k+1} (z_j + 1) k \sum_{i=1}^{k+1} \frac{z_j}{z_j + 1}$$

which illustrates that the induction hypothesis is true for $(k + 1)$, and consequently, the lemma is true for each dimension $m \geq 1$. $\qquad \square$

6

Density function of the eigenvalues

General properties of the density function of eigenvalues are studied. Most articles in this chapter implicitly assume the eigenvalues of the adjacency matrix A. Especially for large graphs and random graphs, the density function is more suitable than the list of eigenvalues.

6.1 Definitions

121. The density function of the eigenvalues $\{\lambda_m\}_{1 \leq m \leq N}$ is, by definition,

$$f_\lambda(t) = \frac{1}{N} \sum_{m=1}^{N} \delta(t - \lambda_m) \tag{6.1}$$

where $\delta(t)$ is the Dirac function, which can be written as a complex integral

$$\delta(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{zt} dz \qquad (c > 0)$$

Hence, we have for $c > 0$,

$$f_\lambda(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{zt} \varphi_\lambda(z) \, dz \tag{6.2}$$

where, analogous to the definition of a probability generating function,

$$\varphi_\lambda(z) = \frac{1}{N} \sum_{m=1}^{N} \exp(-z\lambda_m) \tag{6.3}$$

can be interpreted as the generating function of the density function of the eigenvalues $\{\lambda_m\}_{1 \leq m \leq N}$.

122. In fact, $\varphi_\lambda(z)$ is a general Dirichlet series (Hardy and Riesz, 1964). Summing

$$\lambda_m^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty x^{s-1} e^{-\lambda_m x} dx$$

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over m gives

$$\sum_{m=1}^{N} e^{-s\log\lambda_m} = \frac{1}{\Gamma(s)} \int_0^{\infty} x^{s-1} \sum_{m=1}^{N} e^{-\lambda_m x} dx$$

which relates the general Dirichlet series on the set $\{\lambda_m\}_{1\leq m\leq N}$ by a Mellin transform to that on the set $\{\log\lambda_m\}_{1\leq m\leq N}$. By inverse Mellin transform, we thus find an alternative expression for (6.3),

$$\varphi_\lambda(z) = \frac{1}{2\pi N i} \int_{c^*-i\infty}^{c^*+i\infty} \Gamma(s) \sum_{m=1}^{N} e^{-s\log\lambda_m} z^{-s} ds$$

where $c^* > 0$. By closing the contour over the negative half $\mathrm{Re}(s)$ plane, we obtain the Taylor expansion of (6.3) around zero. Hence, only if $\sum_{m=1}^{N} e^{-s\log\lambda_m}$ can be summed in contrast to $\sum_{m=1}^{N} e^{-\lambda_m x}$, interesting insight may be gained. Formal substitution into (6.2) yields

$$f_\lambda(t) = \frac{1}{(2\pi i)^2 N} \int_{c-i\infty}^{c+i\infty} dz \int_{c^*-i\infty}^{c^*+i\infty} ds \, z^{-s} e^{zt} \Gamma(s) \sum_{m=1}^{N} e^{-s\log\lambda_m}$$

$$= \frac{1}{2\pi i N} \int_{c^*-i\infty}^{c^*+i\infty} ds \left[\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} z^{-s} e^{zt} dz \right] \Gamma(s) \sum_{m=1}^{N} e^{-s\log\lambda_m}$$

Using Hankel's contour integral (see Abramowitz and Stegun (1968, Section 6.1.4); Sansone and Gerretsen (1960, p. 202)), the integral between brackets equals

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} z^{-s} e^{zt} dz = \frac{t^{s-1}}{\Gamma(s)}$$

Hence, besides (6.2), $f_\lambda(t)$ can be expressed as an inverse Mellin transform

$$f_\lambda(t) = \frac{1}{2\pi i N} \int_{c^*-i\infty}^{c^*+i\infty} ds \, t^{s-1} \sum_{m=1}^{N} e^{-s\log\lambda_m}$$

of $\frac{1}{N} \sum_{m=1}^{N} e^{-s\log\lambda_m}$.

123. Another integral form can be derived by applying Abel summation. The result (Hardy and Riesz, 1964) is

$$\varphi_\lambda(z) = z \int_{\lambda_N}^{\lambda_1} A_\lambda(u) e^{-uz} du + e^{-\lambda_1 z}$$

where

$$A_\lambda(t) = \frac{1}{N} \sum_{\lambda_m < t} 1$$

$$= \frac{N-m}{N} \qquad \text{if } \lambda_{m+1} \leq t < \lambda_m$$

which is, in terms of probability theory, nothing else than $\Pr\left[\lambda \le t\right] = F_\lambda(t) = \int_{\lambda_N}^t f_\lambda(u)\,du$.

124. A noteworthy relation, based on (8.7) in **art. 138**, is

$$\varphi_\lambda(z) = \frac{1}{N}\text{trace}\left(e^{-zA}\right) \tag{6.4}$$

because, if $\{\lambda_m\}_{1 \le m \le N}$ are the eigenvalues of a symmetric matrix $A_{N \times N}$, then $\{e^{-z\lambda_m}\}_{1 \le m \le N}$ are the eigenvalues of e^{-zA}. Indeed, since $e^{-zA} = \sum_{k=0}^\infty \frac{A^k}{k!}(-z)^k$ and $A^k = X\text{diag}(\lambda_m^k)X^T$, where the orthogonal matrix X has the eigenvectors of A as columns (**art. 151**), we have that

$$e^{-zA} = X\text{diag}\left(e^{-z\lambda_m}\right)X^T$$

The argument shows, in addition, that the eigenvector of A belonging to the eigen value λ_m is also the eigenvector of e^{-zA} belonging to the eigenvalue $e^{-z\lambda_m}$. The relation with a probability generating function, $\varphi_\lambda(z) = E\left[e^{-z\lambda}\right]$, suggests that the moments $E\left[\lambda^n\right] = (-1)^n \varphi_\lambda^{(n)}(0)$, and with (6.4) that

$$E\left[\lambda^n\right] = \frac{1}{N}\text{trace}\left(A^n\right) \tag{6.5}$$

This relation lies at the basis of Wigner's moment approach (**art. 135**) to computing the eigenvalues of random matrices.

6.2 The density when $N \to \infty$

125. Since e^{-z} is convex for real z, an application of the general convexity bound (Van Mieghem, 2006b, eq. (5.3)), from which Jensen's inequality is also derived, gives

$$\varphi_\lambda(z) = \frac{1}{N}\sum_{m=1}^N \exp\left(-z\lambda_m\right) \ge \exp\left(-\frac{z}{N}\sum_{m=1}^N \lambda_m\right) = 1$$

where we have used that $\sum_{m=1}^N \lambda_m = 0$ for the adjacency matrix A (**art. 25**).

126. The basic summation formula (Titchmarsh and Heath Brown, 1986, p. 13),

$$\sum_{a < k \le b} f(k) = \int_a^b f(x)\,dx + \int_a^b \left(x - [x] - \frac{1}{2}\right)\frac{df(x)}{dx}\,dx + \left(a - [a] - \frac{1}{2}\right)f(a)$$
$$- \left(b - [b] - \frac{1}{2}\right)f(b) \tag{6.6}$$

is valid for any function $f(x)$ with continuous derivative in the interval $[a, b]$. We define the continuous function $\Lambda(x)$ on $[0, N]$ such that $\Lambda(m) = \lambda_m$ by Lagrange interpolation (**art. 206**). Since, for any $m \in [1, N]$, **art. 23** shows that $-(N-1) < \lambda_m \le N-1$ and since $\lambda_N \le \lambda_{N-1} \le \ldots \le \lambda_1$, $|\Lambda(x)|$ is bounded on $[1, N]$ by $N-1$

and $\Lambda(m) \leq \Lambda(m-1)$ for any m. Thus, $\Lambda(x)$ is continuous and not increasing on $[0, N]$. Application of (6.6) yields

$$\varphi_\lambda(z) = \frac{1}{N} \int_0^N e^{-z\Lambda(x)} dx - y_N(z) + \frac{e^{-z\Lambda(N)} - e^{-z\Lambda(0)}}{2N}$$

where

$$y_N(z) = \frac{z}{N} \int_0^N \left(x - [x] - \frac{1}{2}\right) e^{-z\Lambda(x)} \frac{d\Lambda(x)}{dx} dx$$

Since $-\frac{1}{2} \leq x - [x] - \frac{1}{2} \leq \frac{1}{2}$ and $\frac{d\Lambda(x)}{dx} \leq 0$, we may bound $y_N(z)$ for real z as,

$$\frac{z}{2N} \int_0^N e^{-z\Lambda(x)} \frac{d\Lambda(x)}{dx} dx \leq y_N(z) \leq -\frac{z}{2N} \int_0^N e^{-z\Lambda(x)} \frac{d\Lambda(x)}{dx} dx$$

With

$$\int_0^N e^{-z\Lambda(x)} \frac{d\Lambda(x)}{dx} dx = \int_{\Lambda(0)}^{\Lambda(N)} e^{-z\Lambda(x)} d\Lambda(x) = \frac{e^{-z\Lambda(0)} - e^{-z\Lambda(N)}}{z}$$

we have that

$$\frac{e^{-z\Lambda(0)} - e^{-z\Lambda(N)}}{2N} \leq y_N(z) \leq \frac{e^{-z\Lambda(N)} - e^{-z\Lambda(0)}}{2N}$$

such that, for real z,

$$\frac{1}{N} \int_0^N e^{-z\Lambda(x)} dx \leq \varphi_\lambda(z) \leq \frac{1}{N} \int_0^N e^{-z\Lambda(x)} dx + \frac{e^{-z\Lambda(N)} - e^{-z\Lambda(0)}}{N}$$

The density function $f_\lambda(t)$ involves a line integration (6.2) over $\mathrm{Re}(z) = c > 0$. If, for $\mathrm{Re}(z) > 0$,

$$\lim_{N\to\infty} \frac{e^{-z\Lambda(N)} - e^{-z\Lambda(0)}}{N} = \lim_{N\to\infty} \frac{e^{-z\Lambda(N)}}{N} = 0$$

then the limit

$$\lim_{N\to\infty} \varphi_\lambda(z) = \lim_{N\to\infty} \frac{1}{N} \int_0^N e^{-z\Lambda(x)} dx$$

exists and, hence, also $\lim_{N\to\infty} f_\lambda(t)$. The condition means that the absolute value of the smallest eigenvalue $\Lambda(N) = \lambda_N < 0$ grows as $|\lambda_N| = O(\log N)$ at most, for $\mathrm{Re}(z) = c > 0$, but arbitrarily small. This condition is quite restrictive and suggests to consider the spectrum of all *normalized* eigenvalues.

127. We start from $E[\lambda^m] = \frac{1}{N}\mathrm{trace}(A^m)$ and using the Stieltjes integral (**art. 241**),

$$E[\lambda^m] = \int_{-\infty}^{\infty} x^m dF_\lambda(G_N) = \frac{1}{N}\mathrm{trace}\left(A_{N\times N}^m\right)$$

If $\lim_{N\to\infty} \frac{1}{N}\mathrm{trace}\left(A_{N\times N}^m\right) = w_G(m)$ exists, then

$$\int_{-\infty}^{\infty} x^m dF_{\lambda\infty} = w_G(m) \qquad (6.7)$$

which implies that the limiting distribution $F_{\lambda\infty}$ of the eigenvalues of $G_\infty = \lim_{N\to\infty} G_N$ exists. Assuming that this distribution is also differentiable, then $\int_\infty^\infty x^m dF_{\lambda\infty} = \int_\infty^\infty x^m f_{\lambda\infty}(x)\,dx$. Since $\text{trace}(A_{N\times N}) = 0$ and $\text{trace}(A_{N\times N}^2) = 2L$, we find, beside $\int_\infty^\infty f_{\lambda\infty}(x)\,dx = 1$, that

$$\int_\infty^\infty x f_{\lambda\infty}(x)\,dx = 0$$

$$\int_\infty^\infty x^2 f_{\lambda\infty}(x)\,dx = E[D]$$

Multiplying both sides in (6.7) by $\frac{(-z)^m}{m!}$ and summing over all integers m yields again the pgf

$$\varphi_{\lambda\infty}(z) = \int_\infty^\infty e^{-zx} dF_{\lambda\infty} = \sum_{m=0}^\infty \frac{(-z)^m}{m!} w_G(m) \tag{6.8}$$

6.3 Examples of spectral density functions

128. Applying (6.3) to the $N-1$ hops path using (5.8) yields

$$\varphi_{\lambda_P}(z) = \frac{1}{N}\sum_{k=1}^N \exp\left(-2z\cos\left(\frac{\pi k}{N+1}\right)\right)$$

Since $\Lambda(x) = 2\cos\left(\frac{\pi x}{N+1}\right)$ and

$$\lim_{N\to\infty} \frac{e^{-z\Lambda(N)}}{N} = \lim_{N\to\infty} \frac{e^{-2z\cos\left(\frac{\pi N}{N+1}\right)}}{N} = 0$$

art. 126 shows that the limit generating function exists,

$$\lim_{N\to\infty}\varphi_\lambda(z) = \lim_{N\to\infty} \frac{1}{N}\int_0^N e^{-2z\cos\left(\frac{\pi x}{N+1}\right)} dx$$

$$= \lim_{N\to\infty} \frac{N+1}{N\pi}\int_0^{\frac{\pi N}{N+1}} e^{-2z\cos\theta} d\theta$$

Hence,

$$\lim_{N\to\infty}\varphi_{\lambda_P}(z) = \frac{1}{\pi}\int_0^\pi \exp\left(-2z\cos\theta\right) d\theta = I_0\left(-2z\right) = I_0\left(2z\right)$$

where $I_n(z)$ is the modified Bessel function (Abramowitz and Stegun, 1968, Section 9.6.19). The inverse Laplace transform is

$$\lim_{N\to\infty} f_\lambda(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{zt} I_0\left(2z\right) dz = \frac{1}{2\pi^2 i}\int_{c-i\infty}^{c+i\infty} e^{z(t+2)}\left\{\pi e^{-2z} I_0\left(2z\right)\right\} dz$$

and with the Laplace pair in Abramowitz and Stegun (1968, Section 29.3.124), we arrive at the spectral density function of an infinitely long path:

$$\lim_{N \to \infty} f_\lambda(t) = \frac{1}{\pi} \frac{1}{\sqrt{4 - t^2}} 1_{|t| < 2} \tag{6.9}$$

129. The spectrum of an arbitrary path in a graph with N nodes can be computed if the distribution of the hopcount $H_N > 0$ of that path is known. Indeed, using the law of total probability yields

$$\Pr[\lambda_{\text{arbitrary path}} \leq t] = \sum_{k=1}^{N-1} \Pr[\lambda_{\text{arbitrary path}} \leq t \,|\, H_N = k] \Pr[H_N = k]$$

$$= \sum_{k=1}^{N-1} \Pr[\lambda_{k\text{-hop path}} \leq t] \Pr[H_N = k]$$

Differentiation gives us the density,

$$f_{\lambda_{\text{arbitrary path}}}(t) = \sum_{k=1}^{N-1} f_{\lambda_{k \text{ hop path}}}(t) \Pr[H_N = k]$$

Introducing the definition (6.1) combined with the spectrum specified in Section 5.5,

$$f_{\lambda_{k \text{ hop path}}}(t) = \frac{N - k - 1}{N} \delta(t) + \frac{1}{N} \sum_{m=1}^{k+1} \delta\left(t - 2\cos\left(\frac{\pi m}{k + 2}\right)\right)$$

gives

$$f_{\lambda_{\text{arbitrary path}}}(t) = \frac{N - 1 - E[H_N]}{N} \delta(t)$$

$$+ \frac{1}{N} \sum_{k=1}^{N-1} \sum_{m=1}^{k+1} \delta\left(t - 2\cos\left(\frac{\pi m}{k + 2}\right)\right) \Pr[H_N = k]$$

The spectral peak at $t = 0$ has a strength equal to $\frac{N - 1 - E[H_N]}{N}$. Just as for the $N - 1$ hop path, the spectrum lies in the interval $(-2, 2)$ at discrete values $t = 2\cos\left(\frac{\pi m}{k + 2}\right)$ that range over more possible values than a constant hop path. Moreover, the strength or amplitude of a peak is modulated by the hopcount distribution.

130. Applying (6.3) to the small world graph SW_k, with (5.3), gives

$$\varphi_{\lambda_{\text{SW } k}}(z) = \frac{e^z}{N} \sum_{m=1}^{N} \exp\left(-z \frac{\sin\left(\frac{\pi(m-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(m-1)}{N}\right)}\right)$$

$$= \frac{e^z}{N} \sum_{m=0}^{N-1} \exp\left(-z \frac{\sin\left(\frac{\pi m(2k+1)}{N}\right)}{\sin\left(\frac{\pi m}{N}\right)}\right)$$

Since $\Lambda(x) = \frac{\sin\left(\frac{\pi(x-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(x-1)}{N}\right)} - 1$ and $\Lambda(N) = \frac{\sin\left(\frac{\pi(N-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(N-1)}{N}\right)} - 1 \geq (\lambda_{\mathrm{SW}k})_{\min}$,

which is independent of N, the limit generating function exists

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k}}(z) = \lim_{N\to\infty} \frac{e^z}{N} \int_0^N \exp\left(-z \frac{\sin\left(\frac{\pi(x-1)(2k+1)}{N}\right)}{\sin\left(\frac{\pi(x-1)}{N}\right)}\right) dx$$

$$= \lim_{N\to\infty} \frac{e^z}{\pi} \int_{\frac{\pi}{N}}^{\frac{\pi(N-1)}{N}} \exp\left(-z \frac{\sin(2k+1)\theta}{\sin\theta}\right) d\theta$$

Thus,

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k}}(z) = \frac{e^z}{\pi} \int_0^\pi \exp\left(-z \frac{\sin(2k+1)\theta}{\sin\theta}\right) d\theta \tag{6.10}$$

In terms of the Chebyshev polynomial $U_n(x)$ of the second kind,

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k}}(z) = \frac{e^z}{\pi} \int_0^\pi \exp\left(-z U_{2k}(\cos\theta)\right) d\theta$$

Since $\frac{\sin(2k+1)x}{\sin x} = \frac{\sin(2k+1)(\pi-x)}{\sin(\pi-x)}$, the definition (5.4) shows that $U_{2k}(\cos\theta) = U_{2k}(\cos((\pi-\theta)))$. Hence,

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k}}(z) = \frac{2e^z}{\pi} \int_0^{\frac{\pi}{2}} \exp\left(-z U_{2k}(\cos\theta)\right) d\theta \tag{6.11}$$

We return to the generating function (6.10). With $U_{2k}(\cos\theta) = \frac{\sin(2k+1)\theta}{\sin\theta} = 1 + 2\sum_{j=1}^k \cos 2j\theta$, we have

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k}}(z) = \frac{1}{\pi} \int_0^\pi \exp\left(-2z \sum_{j=1}^k \cos 2j\theta\right) d\theta$$

If $k = 1$, we find after some manipulations that $\frac{1}{\pi} \int_0^\pi \exp\left(-2z\cos 2\theta\right) d\theta = I_0(2z)$, which shows that the limit density of the infinite cycle ($k = 1$) is the same as that (6.9) of the infinite path.

For $k = 2$, we find

$$\lim_{N\to\infty} \varphi_{\lambda_{\mathrm{SW}k=2}}(z) = \frac{1}{\pi} \int_0^\pi e^{-2z\cos 2\theta} e^{-2z\cos 4\theta} d\theta$$

Applying the generating function (Abramowitz and Stegun, 1968, Section 9.6.34) of the modified Bessel function,

$$e^{z\cos x} = I_0(z) + 2\sum_{j=1}^\infty I_j(z) \cos(jx)$$

to $e^{2z\cos 4\theta}$ gives

$$\lim_{N\to\infty} \varphi_{\lambda_{\text{SW}k\ 2}}(z) = I_0(2z)\frac{1}{\pi}\int_0^\pi e^{2z\cos 2\theta}d\theta$$

$$+ 2\sum_{j=1}^\infty (-1)^j I_j(2z)\frac{1}{\pi}\int_0^\pi e^{2z\cos 2\theta}\cos(4j\theta)\,d\theta$$

Using (Abramowitz and Stegun, 1968, Section 9.6.19)

$$I_n(z) = \frac{1}{\pi}\int_0^\pi e^{z\cos x}\cos nx\ dx$$

yields

$$\lim_{N\to\infty} \varphi_{\lambda_{\text{SW}k\ 2}}(z) = I_0^2(2z) + 2\sum_{j=1}^\infty (-1)^j I_j(2z) I_{2j}(2z)$$

The inverse Laplace transform is

$$\lim_{N\to\infty} f_{\lambda_{\text{SW}k\ 2}}(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{zt}\left\{ I_0^2(2z) + 2\sum_{j=1}^\infty (-1)^j I_j(2z) I_{2j}(2z)\right\}dz$$

We cannot evaluate this integral in closed form.

6.4 Density of a sparse regular graph

We present here an ingenious way of McKay (1981), who succeeded in finding the asymptotic density of the eigenvalues of the adjacency matrix of a regular, sparse graph.

131. *A large sparse, regular graph.* Consider a regular graph $G(r; N)$, where each node has degree r. The sparseness of $G(r; N)$ is here understood in the sense that $G(r; N)$ has a local tree like structure. In other words, for small enough integers h, the graph induced by the nodes at hop distance $1, 2, \ldots, h$ from a certain node n is a tree, more specific a k ary, regular tree with the out degree $k = r - 1$. We will first determine the moments via trace(A^m), as explained in **art.** 127, where each element $(A^m)_{jj}$ equals the number of closed walks of m hops starting at node j and returning at j (**art.** 17). In view of the regularity of $G(r; N)$, it is expected that, for $N \to \infty$,

$$\frac{1}{N}\text{trace}(A^m) = \frac{1}{N}\sum_{j=1}^N (A^m)_{jj} \to (A^m)_{nn}$$

Hence, for large N and fixed m, the local structure around any node n is almost the same. In addition, as long as the contribution $c(N)$ of cycles to trace(A^m) is small, i.e., $c(N) = o(N)$, the above limit is unaltered, for $\frac{1}{N}\left(\sum_{j=1}^N (A^m)_{jj} \pm c(N)\right) \to$

$(A^m)_{nn}$. The fact that the number of cycles in $G(r; N)$ grows less than propor tionally with N is an alternative way to define the sparseness of $G(r; N)$.

132. *Random walks and the reflection principle.* McKay (1981) had the fortu nate idea to relate the computation of the number of closed walks to the powerful reflection principle, primarily used in the theory of random walks.

The largest hop distance reached in a k ary tree by a closed walk of m hops is $\left[\frac{m}{2}\right]$. The length m of all closed walks in a k ary tree is even. Moreover, all walks travel some hops down and return along the same path back to the root n. Due to the regular structure, the analogy with a path in a simple random walk is very effective.

In a *simple random walk*, an item moves along the (vertical) x axis over the integers during n epochs, measured along the horizontal k axis. At each epoch k, the item jumps either one step to the right ($x_k = x_{k\ 1} + 1$) or one step to the left ($x_k = x_{k\ 1} - 1$). Assuming that the item starts at the origin at epoch 0, then $x_0 = 0$, his position at $k = n$ equals $x_n = r - l$, where r and l are the total number of right and left steps, respectively. Geometrically, plotting the x distance versus discrete time k, the sequence $x_1, x_2, \ldots, x_n$ represents a path from the origin to the point (n, x_n). The number of such paths with r right steps is $\binom{n}{r} = \binom{n}{n\ r} = \binom{n}{l}$, which is thus equal the number of paths with l left steps, because $l + r = n$. Also, since $r = \frac{x+n}{2}$ we write in the sequel x for x_n the number of paths from the origin to the point (n, x) is

$$T_{(n,x)} = \binom{n}{\frac{x+n}{2}} 1_{\left\{\frac{x+n}{2} \in \mathbb{N}\right\}} \tag{6.12}$$

In general, it is clear that x_k can be either negative, positive or zero. The reflection principle states that:

Theorem 29 (Reflection principle) *The number of paths from the point $a = (m, |x|)$ to the point $b = (n, |y|)$ that cross or touch the k axis is equal to the number of all paths from $-a = (m, -|x|)$ to that same point b.*

The reflection of a point (t, x) is the point $(t, -x)$.

Proof: The reflection principle is demonstrated by showing a one to one cor respondence with the subpath from $a = (m, |x|)$ to $c = (\mu, 0)$ and the reflected subpath from $-a = (m, -|x|)$ to c. For each subpath from a to c, there corre sponds precisely one subpath from $-a$ to c (and the sequel of c to b is the same in both cases). $\square$

A direct consequence of Theorem 29 is the so called ballot theorem:

Theorem 30 (Ballot) *The number of paths from the origin to (n, x), where $n, x \in \mathbb{N}_0$, that never touch the discrete time k axis equals $\frac{x}{n} T_{(n,x)}$.*

Never touching the x axis implies that $x_1 > 0, x_2 > 0, \ldots, x_n = x > 0$. The proof is too nice to not include.

Proof: Since $x_1 > 0$, the first step in such a path is necessarily the point $(1,1)$. Hence, the number of paths from the origin above the k axis to the point (n,x) is equal to the number of paths from $(1,1)$ to (n,x) lying above the k axis. By the reflection principle and (6.12), that number equals $T_{(n\ 1,x\ 1)} - T_{(n\ 1,x+1)} = \frac{x}{n}T_{(n,x)}$. $\qquad\square$

With this preparation, we can determine $(A^m)_{nn}$. Each walk of m hops can be represented by the sequence of points $(1,1), (2, h_2), \ldots (m, h_m)$, where $h_j \geq 0$ is the distance in hops from the root node n. A closed walk means that $h_m = 0$. Each such walk of m steps may consist of smaller walks l, each time when $h_j = 0$ for $0 < j < m$. In the language of a random walk, each time that the path from the origin back to the origin and only lying above the k axis, touches the k axis at $(j, h_j = 0)$. We thus need to compute the number such paths with l points touching the k axis. Feller (1970, pp. 90 91) proves that this number of paths equals $\frac{l}{m\ l}\binom{m}{\left[\frac{m}{2}\right]}1_{\{\frac{m}{2}\in\mathbb{N}\}}$. An elementary closed walk $c \in [1, s]$ consists of one excursion to some maximum level H_c and back along the same track. If there is more than one maximum, then H_c denotes the sum of these maxima. The total number of such elementary closed walks c is $r(r-1)^{H_c\ 1}$ because the root has degree r, and from hop level 1 on, each node has outdegree $r - 1$. Only the upwards steps towards the local maxima contribute to the determination of the total number of walks in a type c walk. Since there are s such elementary closed walks, their total is $\prod_{c=1}^{l} r(1-r)^{H_c\ 1} = r^l (r-1)^{\ l}(r-1)^{\sum_c^l\ 1\ H_c}$. Now, each closed walk has an even number of hops and precisely as many up as down in the k ary tree. Hence, $\sum_{c=1}^{l} H_c = \left[\frac{m}{2}\right]$, the highest possible level to be reached. Thus, we end up with a total of $\frac{l}{m\ l}\binom{m}{\left[\frac{m}{2}\right]}1_{\{\frac{m}{2}\in\mathbb{N}\}}r^l(r-1)^{\left[\frac{m}{2}\right]\ l}$ walks with l touching points. Finally, summing over all possible of l yields McKay's basic result

$$\left(A^{2m}\right)_{nn} = \sum_{l=1}^{m} \binom{2m-l}{m}\frac{l}{2m-l}r^l(r-1)^{m\ l} \qquad (6.13)$$

$$\left(A^{2m+1}\right)_{nn} = 0$$

133. *Asymptotic density $f_{\lambda\infty}(x)$.* The next hurdle is the inversion of (6.7) in **art.** 127. We assume that the limit density exists and is differentiable such that

$$\int_{\infty}^{\infty} x^{2m} f_{\lambda\infty}(x)\, dx = \sum_{l=1}^{m}\binom{2m-l}{m}\frac{l}{2m-l}r^l(r-1)^{m\ l}$$

and $f_{\lambda\infty}(x) = f_{\lambda\infty}(-x)$ is even to satisfy $\left(A^{2m+1}\right)_{nn} = 0$. Recall from Theorems 21 and 22 that symmetry in the spectrum of A is the unique fingerprint of a bipartite structure of which a tree is a special case. McKay succeeded in finding $f_{\lambda\infty}(x)$ by inverting this relation, using a rather complicated method.
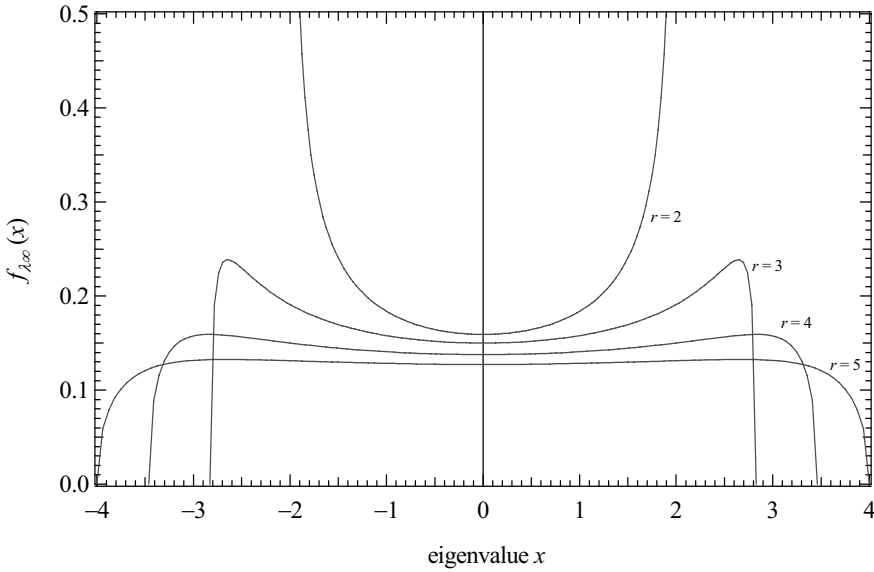
Fig. 6.1. The spectral density $f_{\lambda\infty}(x)$ of a large sparse regular graph for various values of the degree r.

He presents various alternative sums of (6.13) without derivation. Then he derives an asymptotic form of (6.13) for large m to conclude that the extent of $f_{\lambda\infty}(x)$ is bounded, i.e., $f_{\lambda\infty}(x)$ exists only for $|x| \leq 2\sqrt{r-1}$. After normalizing the x range to the interval $[-1, 1]$, he employs Chebyshev polynomials and their orthogonality properties to execute the inversion, resulting in:

Theorem 31 (McKay's Law) *The asymptotic density $f_{\lambda\infty}(x)$ of the eigenvalues of the adjacency matrix of a large, sparse regular graph with degree r equals*

$$f_{\lambda\infty}(x) = \frac{r\sqrt{4(r-1) - x^2}}{2\pi(r^2 - x^2)} 1_{\{|x| \leq 2\sqrt{r-1}\}} \tag{6.14}$$

This spectral density (6.14) is plotted in Fig. 6.1. For $r = 2$, we again find the spectral density of an infinitely long path (6.9).

6.5 Random matrix theory

134. Random matrix theory investigates the eigenvalues of an $N \times N$ matrix A whose elements a_{ij} are random variables with a given joint distribution. Even in case all elements a_{ij} are independent, there does not exist a general expression for the distribution of the eigenvalues. However, in some particular cases (such as Gaussian elements a_{ij}), there exist nice results. Moreover, if the elements a_{ij} are properly scaled, in various cases the spectrum in the limit $N \to \infty$ seems to

converge rapidly to a deterministic limit distribution. The fascinating results of random matrix theory and applications from nuclear physics to the distributions of the non trivial zeros of the Riemann Zeta function are overviewed by Mehta (1991). Recent advances in random matrix theory, discussed by Edelman and Raj Rao (2005), present a general framework that relates, among others, the laws of Wigner (Theorem 32), McKay (Theorem 31) and Marčenko Pastur (Theorem 34) to Hermite, Jacobi and Laguerre orthogonal polynomials (see Chapter 10), respectively. A rigorous mathematical treatment of random matrix theory has just appeared in Anderson *et al.* (2010).

Random matrix theory immediately applies to the adjacency matrix of the Erdős Rényi random graph $G_p(N)$, where each element a_{ij} is 1 with probability p and zero with probability $1 - p$.

6.5.1 *Wigner's Semicircle Law*

135. Wigner's Semicircle Law is the fundamental result in the spectral theory of large random matrices.

Theorem 32 (Wigner's Semicircle Law) *Let A be a random $N \times N$ real sym metric matrix with independent and identically distributed elements a_{ij} with $\sigma^2 = Var[a_{ij}]$ and denote by $\lambda(A_N)$ an eigenvalue of the set of the N real eigenvalues of the scaled matrix $A_N = \frac{A}{\sqrt{N}}$. The probability density function $f_{\lambda(A_N)}(x)$ tends for $N \to \infty$ to*

$$\lim_{N \to \infty} f_{\lambda(A_N)}(x) = \frac{1}{2\pi\sigma^2}\sqrt{4\sigma^2 - x^2}\,1_{|x| \leq 2\sigma} \qquad (6.15)$$

Since Wigner's first proof (Wigner, 1955) of Theorem 32 and his subsequent gen eralizations (Wigner, 1957, 1958) many proofs have been published. However, none of them is short and easy enough to include here. Wigner's Semicircle Law illus trates that, for sufficiently large N, the distribution of the eigenvalues of $\frac{A}{\sqrt{N}}$ does not depend anymore on the probability distribution of the elements a_{ij}. Hence, Wigner's Semicircle Law exhibits a universal property of a class of large, real sym metric matrices with independent random elements. Mehta (1991) suspects that, for a much broader class of large random matrices, a mysterious yet unknown law of large numbers must be hidden. The adjacency matrix of the Erdős Rényi random graph satisfies the conditions in Theorem 32 with $\sigma^2 = p(1 - p)$ and its eigenval ues (apart from the largest) grow as $O\left(\sqrt{N}\right)$. In order to obtain the finite limit distribution (6.15) scaling by $\frac{1}{\sqrt{N}}$ is necessary.

The moment relation (6.5) for the eigenvalues suggests us to compute the mo ments of Wigner's Semicircle Law (6.15),

$$E[\lambda^n] = \int_{\infty}^{\infty} x^n \lim_{N \to \infty} f_{\lambda(A_N)}(x)\,dx = \frac{1}{2\pi\sigma^2}\int_{2\sigma}^{2\sigma} x^n\sqrt{4\sigma^2 - x^2}dx$$

Thus,

$$E[\lambda^n] = \sigma^n C_n$$

where

$$C_n = \frac{2^{n+1}}{\pi} \int_{-1}^{1} t^n \sqrt{1-t^2}\,dt \qquad (6.16)$$

shows that $E[\lambda^n] = 0$ for odd values of n because of integration of an odd function over an even interval. Using the integral of the Beta function (Abramowitz and Stegun, 1968, Section 6.2.1) for $\mathrm{Re}(z) > 0$ and $\mathrm{Re}(w) > 0$,

$$B(z,w) = \int_0^1 t^{z-1}(1-t)^{w-1}\,dt = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}$$

we find that

$$C_{2k} = \frac{2^{2k+2}}{\pi}\int_0^1 t^{2k}\sqrt{1-t^2}\,dt = \frac{2^{2k+1}}{\pi}\int_0^1 x^{k-\frac12}(1-x)^{\frac12}\,dx$$
$$= \frac{2^{2k+1}}{\pi}\frac{\Gamma\left(k+\frac12\right)\Gamma\left(\frac32\right)}{\Gamma(k+2)}$$

Using the functional equation $\Gamma(z+1) = z\Gamma(z)$, $\Gamma\left(\frac12\right) = \sqrt{\pi}$ and the duplication formula (Abramowitz and Stegun, 1968, Section 6.1.18),

$$\Gamma(2z) = \frac{2^{2z-\frac12}}{\sqrt{2\pi}}\Gamma(z)\Gamma\left(z+\frac12\right)$$

finally gives

$$C_{2k} = \frac{(2k)!}{(k+1)!\,k!} = \frac{\binom{2k}{k}}{k+1}$$

These numbers C_{2k} are known as Catalan numbers (Comtet, 1974). Since all moments uniquely define a probability distribution, the only distribution, whose moments are Catalan numbers, is the semicircle distribution, with density function given by (6.15).

Another derivation of the integral (6.16) is given that avoids the theory of the Gamma function. We can rewrite

$$C_n = \frac{2^{n+1}}{\pi}\int_{-1}^{1} t^n \sqrt{1-t^2}\,dt = -\frac{2^{n+1}}{\pi}\int_{-1}^{1}\frac{-t}{\sqrt{1-t^2}}\left\{t^{n-1}(1-t^2)\right\}dt$$

Recognizing that $\frac{d}{dt}\sqrt{1-t^2} = \frac{-t}{\sqrt{1-t^2}}$, partial integration gives

$$C_n = \frac{2^{n+1}}{\pi}\int_{-1}^{1}\sqrt{1-t^2}\,\frac{d}{dt}\left\{t^{n-1}(1-t^2)\right\}dt$$
$$= \frac{2^{n+1}}{\pi}\int_{-1}^{1}\sqrt{1-t^2}\left\{(n-1)t^{n-2} - (n+1)t^n\right\}dt$$
$$= 2(n-1)C_{n-2} - (n+1)C_n$$

which leads, with $C_0 = 1$ and $C_1 = 0$, to the recursion

$$C_n = \frac{2(n-1)}{n+2} C_{n-2}$$

Iteration gives

$$C_n = 2^p \frac{n-1}{n+2} \frac{n-3}{n} \frac{n-5}{n-2} \cdots \frac{n-(2p-1)}{n-(2p-4)} C_{n-2p}$$

If n is odd, $C_n = 0$ (as found above), while if $n = 2k$ and $p = k$, then

$$C_{2k} = 2^{2k} \frac{2k-1}{2k+2} \frac{2k-3}{2k} \frac{2k-5}{2k-2} \cdots \frac{1}{4}$$

$$= 2^{2k} \frac{2k}{2k} \frac{2k-1}{2k+2} \frac{2k-2}{2k-2} \frac{2k-3}{2k} \frac{2k-4}{2k-4} \frac{2k-5}{2k-2} \cdots \frac{1}{4} = \frac{(2k)!}{(k+1)!k!}$$

which again results in the Catalan numbers.

The Catalan numbers appear in many combinatorial problems (see, e.g., Comtet (1974)). For example, the number of paths in the simple random walk that never cross (but may touch) the k axis and that start from the origin and return to the origin at time $n = 2m$, is deduced from the reflection principle (Theorem 29) as

$$T_{(2m,0)} - T_{(2m,-2)} = \binom{2m}{m} - \binom{2m}{m-1} = C_{2m}$$

Indeed, the number of paths from the origin to $(2m, 0)$ that never cross the k axis equals the total number of paths from the origin to $(2m, 0)$, which is $T_{(2m,0)}$, minus the number of paths from the origin to $(2m, 0)$ that cross the k axis at some point. A path that crosses the k axis, touches the line $x = -1$. Instead of considering the reflection principle with respect to the $x = 0$ line — the k axis —, it evidently applies for a reflection around a line at $x = j \in \mathbb{Z}$. Thus, the number of paths from $(2m, 0)$ to the origin that touch or cross the line at $x = -1$ is equal to the total number of paths from $(2m, -2)$ to the origin. That latter number is $T_{(2m,-2)}$, which demonstrates the claim.

136. A single eigenvalue has measure zero and does not contribute to the limit probability density function (6.15). By using Wigner's method, Füredi and Komlós (1981) have extended Wigner's Theorem 32.

Theorem 33 (Füredi-Komlós) *Let A be a random $N \times N$ real symmetric matrix where the elements $a_{ij} = a_{ji}$ are independent (not necessary identically distributed) random variables bounded by a common bound K. Assume that, for $i \neq j$, these random variables possess a common mean $E[a_{ij}] = \mu$ and common $Var[a_{ij}] = \sigma^2$, while $E[a_{ii}] = \nu$.*
(a) If $\mu > 0$, then the distribution of the largest eigenvalue $\lambda_1(A)$ can be approximated to within order $O\left(\frac{1}{\sqrt{N}}\right)$ by a Gaussian distribution with mean

$$E[\lambda_1(A)] \simeq (N-1)\mu + \nu + \frac{\sigma^2}{\mu}$$

and (bounded) variance

$$Var\left[\lambda_1\left(A\right)\right] \simeq 2\sigma^2$$

In addition, with probability tending to 1,

$$\max_{j>1}\left|\lambda_j\left(A\right)\right| < 2\sigma\sqrt{N} + O\left(N^{1/3}\log N\right) \tag{6.17}$$

(b) *If $\mu = 0$, then all eigenvalues of A, including the largest, obey the last bound (6.17).*

137. *Spectrum of the Erdős Rényi random graph.* We apply the powerful Theorem 33 to the Erdős Rényi random graph $G_p\left(N\right)$. Since $\mu = p$, $\nu = 0$ and $\sigma^2 = p\left(1-p\right)$, Theorem 33 states that the largest eigenvalue λ_1 is a Gaussian random variable with mean $E\left[\lambda_1\right] = \left(N-2\right)p+1+O\left(\frac{1}{\sqrt{N}}\right)$ and $\text{Var}[\lambda_1\left(A\right)] \simeq 2p\left(1-p\right)$, while all other eigenvalues are smaller in absolute value than $2\sqrt{p\left(1-p\right)N} + O\left(N^{1/3}\log N\right)$.
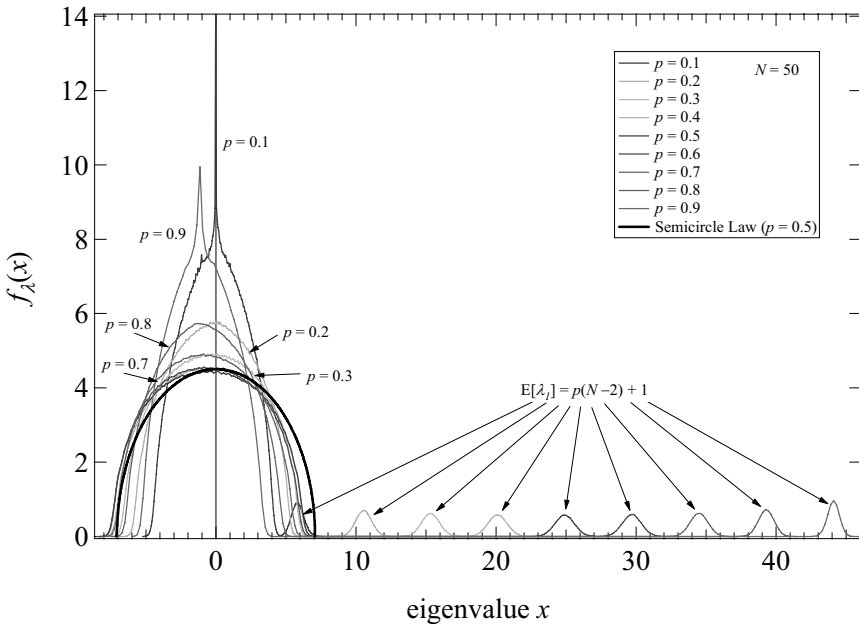
Fig. 6.2. The probability density function of an eigenvalue in $G_p(50)$ for various p. Wigner's Semicircle Law, rescaled and for $p = 0.5$ ($\sigma^2 = \frac{1}{4}$), is shown in bold. We observe that the spectrum for p and $1-p$ is similar, but slightly shifted. The high peak for $p = 0.1$ reflects disconnectivity, while the high peak at $p = 0.9$ shows the tendency to the spectrum of the complete graph where $N-1$ eigenvalues are precisely -1.

The spectrum of $G_p\left(50\right)$ together with the properly rescaled Wigner's Semicircle Law (6.15) is plotted in Fig. 6.2. Already for this small value of N, we observe

that Wigner's Semicircle Law is a reasonable approximation for the intermediate p region. The largest eigenvalue λ_1 for finite N, which is almost Gaussian distributed around $p(N-2)+1$ with variance $2p(1-p)$ by Theorem 33 and shown in Fig. 6.2, but which is not incorporated in Wigner's Semicircle Law, influences the average $E[\lambda] = \frac{1}{N}\sum_{k=1}^{N}\lambda_k = 0$ and causes the major bulk of the pdf around $x = 0$ to shift leftward compared to Wigner's Semicircle Law, which is perfectly centered around $x = 0$.

The finite size variant of the Wigner Semicircle Law for the eigenvalue distribution of the adjacency matrix of the Erdős Rényi random graph $G_p(N)$ is

$$f_\lambda(x) \simeq \frac{\sqrt{4Np(1-p)-(x+p)^2}}{2\pi Np(1-p)}, \quad |x| \le 2p(1-p)\sqrt{N} \qquad (6.18)$$

The expression (6.18) for the bulk density of eigenvalues, thus also ignoring the largest eigenvalue λ_1, agrees very well with simulations for finite N. Below, we sketch the derivation of (6.18). The probabilistic companion of (3.1) is

$$E[\lambda] = \sum_{k=-\infty}^{\infty} k\Pr[\lambda = k] = 0$$

while the discrete random variable λ needs to satisfy

$$\sum_{k=-\infty}^{\infty} \Pr[\lambda = k] = 1$$

The Perron Frobenius Theorem 38 states that any connected graph has one largest eigenvalue λ_1 with multiplicity one, such that $\Pr[\lambda = \lambda_1] = \frac{1}{N}$. Both the mean and the law of total probability can be written, for one realization of an Erdős Rényi random graph, as

$$E[\lambda] = \lambda_1 \frac{1}{N} + \sum_{\text{All others}} k\Pr[\lambda = k] = 0 \qquad (6.19)$$

and

$$\sum_{\text{All others}} \Pr[\lambda = k] = 1 - \frac{1}{N}$$

Fig. 6.2 suggests us to consider the Semicircle Law for finite N shifted over some value ε,

$$f_\lambda(x;\varepsilon) = \frac{\sqrt{4Np(1-p)-(x+\varepsilon)^2}}{2\pi Np(1-p)}, \quad |x| \le 2p(1-p)\sqrt{N}$$

Denoting the radius $R = 2p(1-p)\sqrt{N}$ and passing to the continuous random

variable, relation (6.19) becomes

$$0 = \lambda_1 \frac{1}{N} + \int_{R_\varepsilon}^{R_\varepsilon} x f_\lambda (x; \varepsilon) \, dx$$

$$= \lambda_1 \frac{1}{N} + \int_{R_\varepsilon}^{R_\varepsilon} (x + \varepsilon) f_\lambda (x; \varepsilon) \, dx - \varepsilon \int_{R_\varepsilon}^{R_\varepsilon} f_\lambda (x; \varepsilon) \, dx$$

Since $\int_{R_\varepsilon}^{R_\varepsilon} (x + \varepsilon) f_\lambda (x; \varepsilon) \, dx = 0$ due to symmetry and $\int_{R_\varepsilon}^{R_\varepsilon} f_\lambda (x; \varepsilon) \, dx = 1 - \frac{1}{N}$, we obtain

$$\lambda_1 \frac{1}{N} - \varepsilon \left(1 - \frac{1}{N} \right) = 0$$

Finally, Theorem 33 states that $\lambda_1 = (N - 2) p + O(1)$ such that $\varepsilon = p + O(N^{-1})$ leading to (6.18).
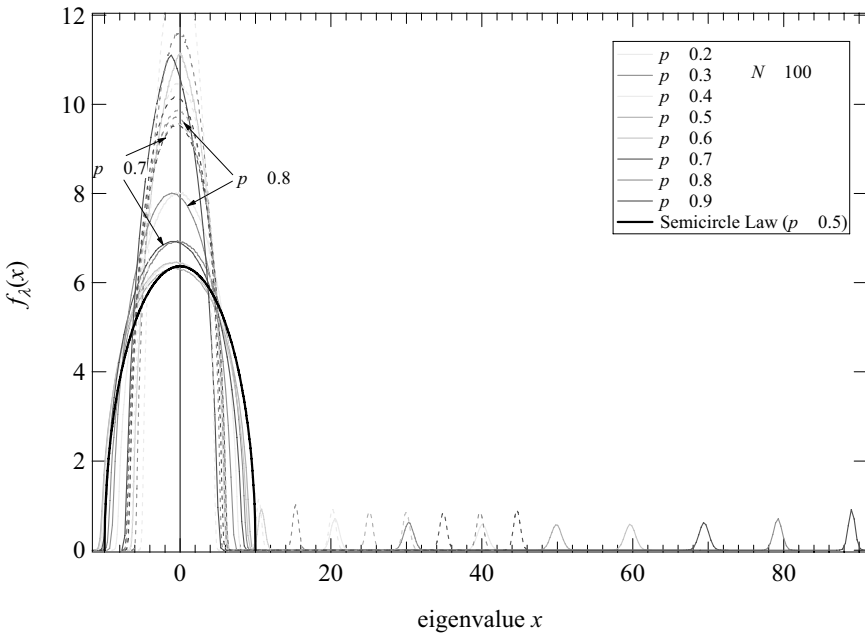
Fig. 6.3. The spectrum of the adjacency matrix of $G_p(100)$ (full lines) and of the corresponding matrix with i.i.d. uniform elements (dotted lines). The small peaks at higher values of x are due to λ_1.

The complement of $G_p(N)$ is $(G_p(N))^c = G_{1-p}(N)$, because a link in $G_p(N)$ is present with probability p and absent with probability $1 - p$ and $(G_p(N))^c$ is also a random graph. For large N, there exists a large range of p values for which both $p \geq p_c$ and $1 - p \geq p_c$ such that both $G_p(N)$ and $(G_p(N))^c$ are connected almost surely. Figure 6.2 shows that the normalized spectra of $G_p(N)$ and $G_{1-p}(N)$ are, apart from a small shift and ignoring the largest eigenvalue, almost identical.

Equation (3.30) indicates that the spectra of a graph and of its complement tend to each other if $\cos \alpha_j \to 0$ (except for the largest eigenvalue which will tend to u). This seems to suggest that $G_p(N)$ and $G_{1-p}(N)$ are tending to a regular graph with degree $p(N-1)$ and $(1-p)(N-1)$ and that these regular graphs (even for small N) have nearly the same spectrum, apart from the largest eigenvalue $p(N-1)$ and $(1-p)(N-1)$ respectively: $\frac{\lambda_{1-p}}{\sqrt{N}} \simeq -\frac{\lambda_p}{\sqrt{N}} - \frac{1}{\sqrt{N}}$ where λ_p is an eigenvalue of $G_p(N)$.

Figure 6.3 shows the probability density function $f_\lambda(x)$ of the eigenvalues of the adjacency matrix A of $G_p(N)$ with $N = 100$ together with the eigenvalues of the corresponding matrix A_U where all one elements in the adjacency matrix of $G_p(100)$ are replaced by i.i.d. uniform random variables on $[0,1]$. Wigner's Semicircle Law provides an already better approximation than for $N = 50$. Since the elements of A_U are always smaller (with probability 1) than those of A, the matrix norm $\|A_U\|_q < \|A\|_q$ and the inequality (8.51) imply that $\lambda_1(A_U) < \lambda_1(A)$. In addition, relation (3.5) shows that $\sum_{k=1}^N \lambda_k^2(A_U) < 2L$ such that $\text{Var}[\lambda(A_U)] < \text{Var}[\lambda(A)]$, which is manifested by a narrower and higher peaked pdf centered around $x = 0$.

6.5.2 The Marčenko-Pastur Law

The last of the classical laws in random matrix theory with an analytic density function for the eigenvalues is given in the next theorem without proof:

Theorem 34 (The Marčenko-Pastur law) *Let C be a random $m \times n$ matrix with independent and identically distributed complex elements c_{ij} with finite $\sigma^2 = Var[c_{ij}]$ and zero mean $E[c_{ij}] = 0$, or the complex elements c_{ij} are independently distributed with a finite fourth order moment. Let $y = \frac{m}{n}$ as $n \to \infty$ and define $a(y) = \sigma^2(1 - \sqrt{y})^2$ and $b(y) = \sigma^2(1 + \sqrt{y})^2$, and denote by $\lambda(S)$ an eigenvalue of the set of the m real eigenvalues of the scaled Hermitian matrix $S = \frac{1}{n}CC^*$. The probability density function $f_{\lambda(S)}(x)$ tends for $n \to \infty$ to*

$$\lim_{n \to \infty} f_{\lambda(S)}(x) = \frac{1_{\{a(y) \le x \le b(y)\}}}{2\pi xy\sigma^2} \sqrt{(x - a(y))(b(y) - x)} + \left(1 - \frac{1}{y}\right) \delta(x) 1_{\{y > 1\}}$$

(6.20)

Marčenko and Pastur (1967) prove Theorem 34 by deriving a first order partial differential equation, from whose solution the unique Stieltjes transform $m(\psi; z)$ of $\psi(x) = \lim_{n \to \infty} f_{\lambda(S)}(x)$ is found. The Stieltjes transform of a function $f(x)$, defined by

$$m(f, z) = \int_\infty^\infty \frac{f(x)}{z - x} dx$$

is essentially a special case of an integral of the Cauchy type, that is treated, together with its inverse, in **art.** 252. This method is essentially different than the

moments method used by McKay (sketched in Section 6.4) and earlier by Wigner (1955).
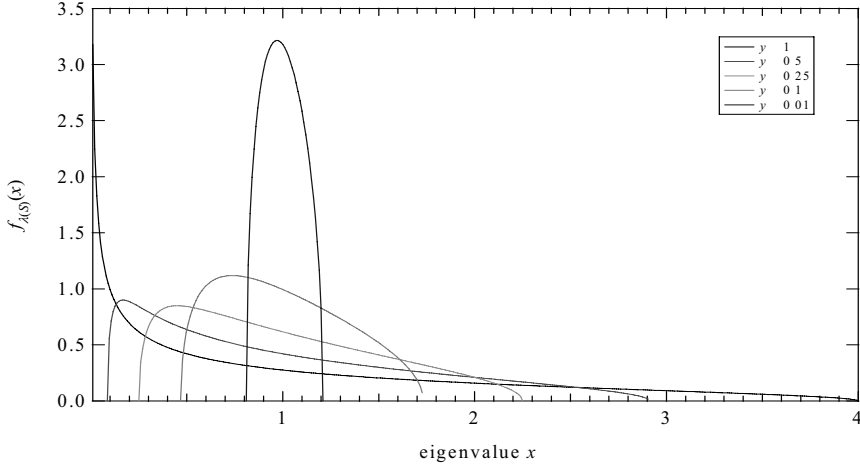
Fig. 6.4. The Marčenko Pastur probability density function (6.20) for various values of y. Each curve starts at $x = a(y)$, which is increasing from 0 to 1 when y decreases from 1 to 0, and ends at $x = b(y)$, which decreases from 4 to 1 when y decreases from 1 to 0. When $y \to 0$, the Marčenko Pastur probability density function tends to a delta function at $x = 1$.

The last term in (6.20), the point mass at $x = 0$, is a consequence of the non square form of C. The rank$(CC^*) \le \min(n, m)$ such, for $y > 1$, the $m \times m$ matrix CC^* has $m - n = m\left(1 - \frac{1}{y}\right)$ zero eigenvalues, while all ny other eigenvalues are the same as those of C^*C, which follows from **art.** 184.

In the case $m = n$ and $y = 1$, and $C = C^T = \frac{A}{\sqrt{n}}$, the eigenvalues of S are the squares of those of $\frac{A}{\sqrt{n}}$. Since the latter eigenvalues obey the Wigner Semicircle Law (6.15) and since the density $f_{X^2}(x) = \frac{f_X(\sqrt{x}) + f_X(-\sqrt{x})}{2\sqrt{x}}$ for any random variable X as shown in Van Mieghem (2006b, p. 50), we find, indeed for $y = 1$, that

$$f_{\lambda(S)} = \frac{f_{\lambda(A_n)}(\sqrt{x}) + f_{\lambda(A_n)}(-\sqrt{x})}{2\sqrt{x}} = \frac{f_{\lambda(A_n)}(\sqrt{x})}{\sqrt{x}}$$

Also, in that case, the matrix S represents a square covariance matrix. In general for m real random $n \times 1$ vectors, S represents the $m \times n$ covariance matrix, that appears in many applications of signal and information theory and physics. Fig. 6.4 illustrates the Marčenko Pastur probability density function $f_{\lambda(S)}(x)$ for various values of $y \le 1$.

7

Spectra of complex networks

This chapter presents some examples of the spectra of complex networks, which we have tried to interpret or to understand using the theory of previous chapters. In contrast to the mathematical rigor of the other chapters, this chapter is more intuitively oriented and it touches topics that are not yet understood or that lack maturity. Nevertheless, the examples may give a flavor of how real world complex networks are analyzed as a sequence of small and partial steps towards (hopefully) complete understanding.

7.1 Simple observations

When we visualize the density function $f_\lambda(x)$ of the eigenvalues of the adjacency matrix of a graph, defined in **art.** 121, peaks at $x = 0$, $x = -1$ and $x = -2$ are often observed. The occurrence of adjacency eigenvalue at those integer values has a physical explanation.

7.1.1 A graph with eigenvalue $\lambda(A) = 0$

A matrix has a zero eigenvalue if its determinant is zero (**art.** 138). A determinant is zero if two rows are identical or if some of the rows are linearly dependent. For example, two rows are identical resulting in $\lambda(A) = 0$, if *two not mutually interconnected nodes are connected to a same set of nodes*. Since the elements a_{ij} of an adjacency matrix A are only 0 or 1, linear dependence of rows occurs every time the sum of a set of rows equals another row in the adjacency matrix. For example, consider the sum of two rows. If node n_1 is connected to the set S_1 of nodes and node n_2 is connected to the distinct set S_2, where $S_1 \cap S_2 = \varnothing$ and $n_1 \neq n_2$, then *the graph has a zero adjacency eigenvalue if another node $n_3 \neq n_2 \neq n_1$ is connected to all nodes in the set $S_1 \cup S_2$.* These two types of zero eigenvalues occur when a graph possesses a "local bipartiteness". In real networks, this type of interconnection often occurs.

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7.1.2 A graph with eigenvalue $\lambda(A) = -1$

An adjacency matrix A has an eigenvalue $\lambda(A) = -1$ every time *a node pair n_1 and n_2 in the graph is connected to a same set S of different nodes and n_1 and $n_2 are mutually also interconnected.* Indeed, without loss of generality, we can relabel the nodes such that $n_1 = 1$ and $n_2 = 2$. In that case, the first two rows in A are of the form

$$
\begin{matrix}
0 & 1 & a_{13} & a_{14} & \cdots & a_{1N} \\
1 & 0 & a_{13} & a_{14} & \cdots & a_{1N}
\end{matrix}
$$

and the corresponding rows in $\det(A - \lambda I)$ of the characteristic polynomial are

$$
\begin{matrix}
-\lambda & 1 & a_{13} & a_{14} & \cdots & a_{1N} \\
1 & -\lambda & a_{13} & a_{14} & \cdots & a_{1N}
\end{matrix}
$$

If two rows are identical, the determinant is zero. In order to make these rows identical, it suffices to take $\lambda = -1$ and $\det(A + I) = 0$, which shows that $\lambda = -1$ is an eigenvalue of A with this particular form. This observation generalizes to a graph where k nodes are fully meshed and, in addition, all k nodes are connected to the same set S of different nodes. Again, we may relabel nodes such that the first k rows describe these k nodes in a complete graph configuration, also called a clique. Let x denote a $(N - k) \times 1$ zero one vector, then ux^T is a matrix with all rows identical and equal to x. The structure of $\det(A - \lambda I)$ is

$$
\det(A - \lambda I) = \left|
\begin{matrix}
(J - (\lambda + 1) I)_{k \times k} & u.x^T \\
B_{(N-k) \times k} & (C - \lambda I)_{(N-k) \times (N-k)}
\end{matrix}
\right|
$$

which shows that the first k rows are identical if $\lambda = -1$, implying that the multiplicity of this eigenvalue is $k - 1$. Observe that the spectrum in Section 5.1 of the complete graph K_N, where $k = N$, indeed contains an eigenvalue $\lambda = -1$ with multiplicity $N - 1$. We can also say that a peak in the density of the adjacency eigenvalues at $\lambda = -1$ reflects that a set of interconnected nodes all have the same neighbors (different from those in the interconnected set).

7.1.3 A graph with eigenvalue $\lambda(A) = -2$

If the graph is a line graph (**art.** 7), then **art.** 9 demonstrates that the adjacency matrix has an eigenvalue equal to $\lambda(A) = -2$ with multiplicity $L - N$. However, it is in general rather difficult to conclude that a graph is a line graph. Each node with degree d locally, a star K_{1d} is transformed in the line graph into a clique with $\binom{d}{2}$ links. Thus, a line graph can be regarded as a collection of interconnected cliques K_{d_j}, where $1 \le j \le N$. The presence of an eigenvalue $\lambda(A) = -2$ is insufficient to deduce that a graph is a line graph. A more elaborate discussion on line graphs is found in Cvetković *et al.* (2009, Section 3.4).

A peak in the density $f_\lambda(x)$ of the eigenvalues of the adjacency matrix at $\lambda(A) = -2$ and $\lambda(A) = 2$ may correspond to a very long path (**art.** 128). As shown in Fig.

6.1, these peaks occur in large, sparse regular graphs with degree $r = 2$ (McKay's Theorem 31).

7.2 Distribution of the Laplacian eigenvalues and of the degree

Although the moments of the Laplacian eigenvalues (**art. 70 72**) can be expressed in terms of those of the degree, in most real world networks the degree distribution and the Laplacian distribution are usually different. In this section, we present a curious example, where both distributions are remarkably alike.

Software is assembled from many interacting units and subsystems at several levels of granularity (subroutines, classes, source files, libraries, etc.) and the inter actions and collaborations of those parts can be represented by a graph, which is called the software collaboration graph. Fig. 7.1 depicts the topology of the VTK network, which represents the collaborations in the VTK visualization C++ library that has been documented and studied by Myers (2003).
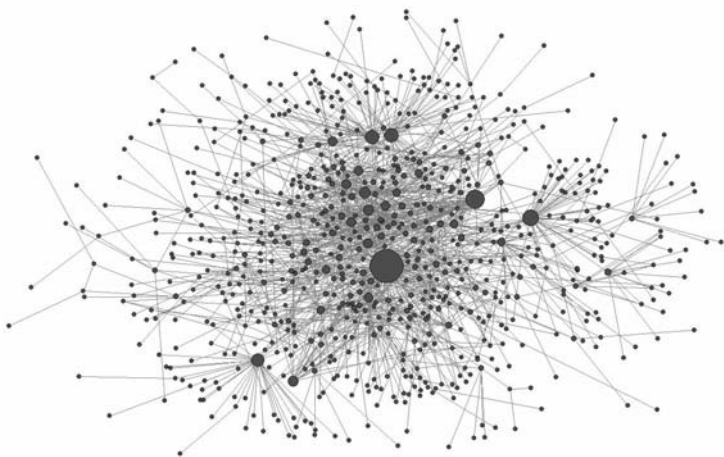
Fig. 7.1. The connected graph of the VTK network with $N = 771$ and $L = 1357$. The nodal size is drawn proportionally to its degree.

Fig. 7.2 shows the correspondence between the degree D and the Laplacian eigen value μ in the connected VTK graph with $N = 771$ nodes, $E[D] = E[\mu] = 3.5201$, $\text{Var}[D] = 33.0603$ and $\text{Var}[\mu] = 36.5804$, which agrees with the theory in **art. 70**. Both the degree D and the Laplacian eigenvalue μ of the VTK graph approximately follow a power law, a general characteristic of many complex networks, and each power law is specified by the fit in the legend in Fig. 7.2, where c_D and c_μ are nor malization constants. The much more surprising fact is that the insert in Fig.7.2

demonstrates how closely the ordered Laplacian eigenvalues μ_k follow the ordered degree $d_{(k)}$. Only in software collaboration networks (such as MySql studied in Myers (2003)), have we observed such a close relationship between D and μ.
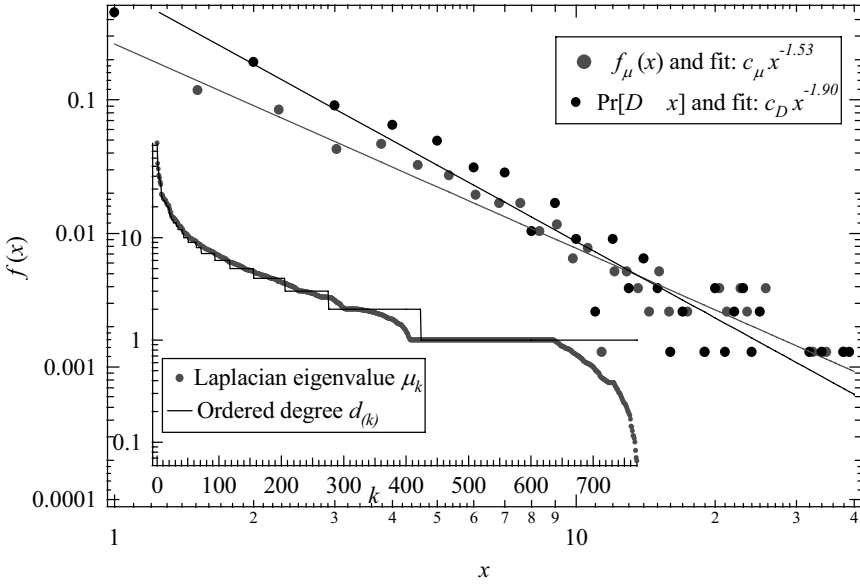
Fig. 7.2. The density function of the degree and of the Laplacian eigenvalues in the soft ware dependence network VTK. The insert shows how close the ordered degree and Lapla cian eigenvalues are.

We do not have an explanation of why D and μ are so close. The observation suggests, in view of the definition of the Laplacian $Q = \Delta - A$, that the influence of the adjacency matrix on the eigenvalues μ of the Laplacian is almost negligible. The bounds in **art. 70**, derived from the interlacing principle,

$$d_{(k)} - \lambda_1(A) \leq \mu_k(Q) \leq d_{(k)} - \lambda_N(A)$$

are too weak because $\lambda_1(A) = 11.46$ and $\lambda_N(A) = -9.13$. Fig. 7.3 presents the density function $f_\lambda(x)$ of the adjacency eigenvalues, which is typically tree like: a high peak $f_\lambda(0) = 0.42$ at the origin $x = 0$ and the density function is almost symmetric around the origin, $f_\lambda(-x) \approx f_\lambda(x)$. If a graph is locally tree like (**art. 131**), we would expect its density to approximately follow McKay's law (Theorem 31) drawn in Fig. 6.1. At first glance, the peaks in $f_\lambda(x)$ at roughly $x = -1$ and $x = 1$ may hint at such a locally tree like structure, but, since the degree r in (6.14) should be at least 2, a locally tree like structure should have peaks at roughly $x = -2$ and $x = 2$. The small variance $\text{Var}[\lambda] = E[D] = 3.52$ (**art. 27**), which is much smaller than $\text{Var}[D]$ and than $\text{Var}[\mu] = \text{Var}[D] + \text{Var}[\lambda]$, supports

the observation above why the adjacency spectrum only marginally influences the Laplacian eigenvalues.
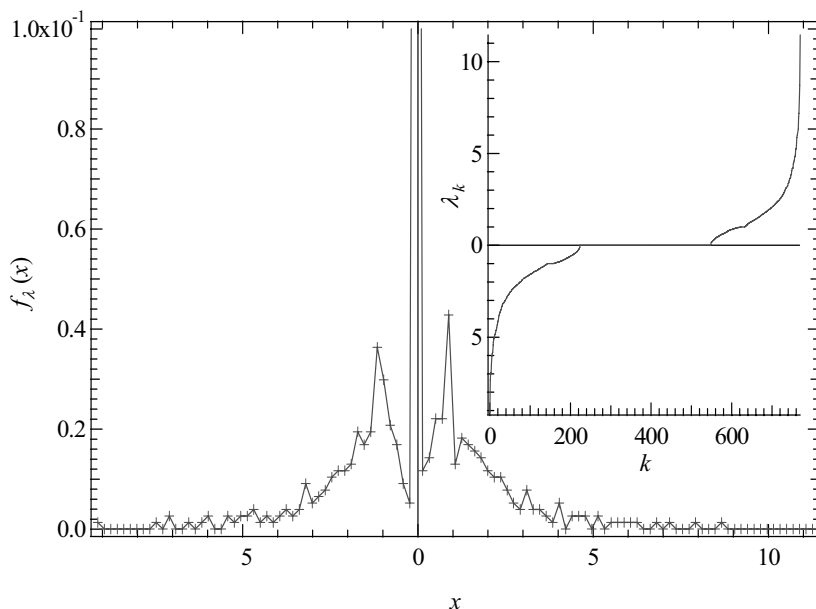
Fig. 7.3. The density of the eigenvalues of the adjacency matrix of the VTK graph. The insert shows the ordered eigenvalues λ_k versus their rank k, where $\lambda_1 = 11.46$ and $\lambda_N = 9.13$.

Finally, we mention the nice estimate of Dorogovtsev *et al.* (2003). Using an ap proximate analysis from statistical physics, but inspired by McKay's result (Section 6.4) based on random walks, Dorogovtsev *et al.* (2003) derived the asymptotic law for the tails of $f_\lambda(x)$ of locally tree like graphs as

$$f_\lambda(x) \approx 2\,|x|\,\mathrm{Pr}\left[D = x^2\right]$$

for large x. For example, in a power law graph where $\mathrm{Pr}\left[D = k\right] = ck^{-\gamma}$, the asymptotic tail behavior of the density function of the adjacency eigenvalues is

$$f_\lambda(x) \approx 2c\,|x|^{1-2\gamma}$$

As shown in Fig. 7.2, the power law exponent for the VTK network is about $\gamma \simeq 1.9$ such that $2\gamma - 1 \simeq 2.8$, but fitting the tail region of $f_\lambda(x)$ in a log log plot gives a slope of -1.7, which again seems to indicate that the VTK graph is not sufficiently close to a locally tree like, power law graph.

7.3 Functional brain network

The interactions between brain areas can be represented by a functional brain net work as shown by Stam and Reijneveld (2007). The concept of functional connec tivity refers to the statistical interdependencies between physiological time series recorded in various brain areas, and is thought to reflect communication between several brain areas. Magneto encephalography (MEG), a recording of the brain's magnetic activity, is a method used to assess functional connectivity within the brain. Each MEG channel is regarded as a node in the functional brain network, while the functional connectivity between each pair of channels is represented by a link, whose link weight reflects the strength of the connectivity, measured via the synchronization likelihood. It is based on the concept of general synchronization (Rulkov *et al.*, 1995), and takes linear as well as nonlinear synchronization between two time series into account. The synchronization likelihood w_{ij} between time se ries i and j lies in the interval $[0, 1]$, with $w_{ij} = 0$ indicating no synchronization, and $w_{ij} = 1$ meaning total synchronization. We adopt the convention that $w_{jj} = 0$, rather than $w_{jj} = 1$, because of the association with the adjacency matrix of the corresponding functional brain graph.
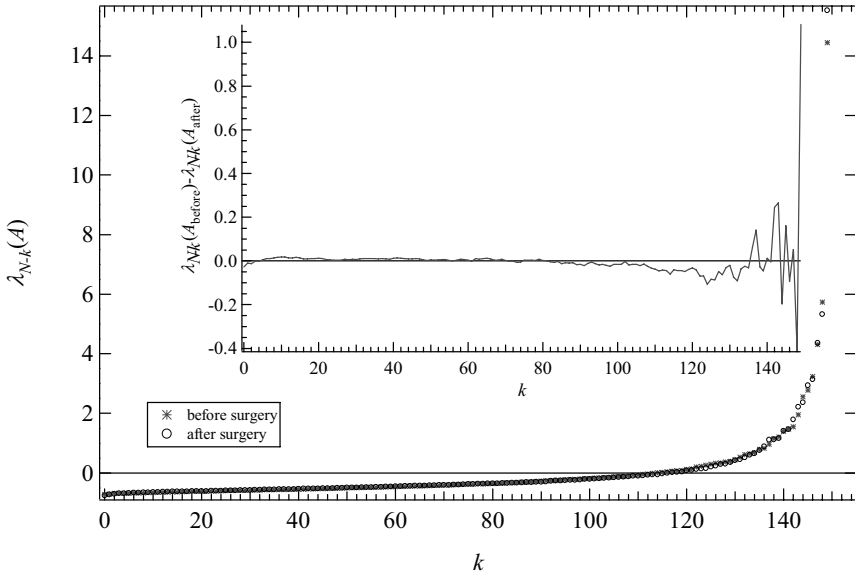
Fig. 7.4. The eigenvalues of the weighted adjacency matrix of the functional brain network before and after surgery in increasing order. The insert shows the differences between the eigenvalues before and after surgery.

The weighted adjacency matrix W of the human functional brain network con tains as elements w_{ij} the synchronization likelihood between the $N = 151$ different MEG channels, each probing a specific area in the human brain as detailed in Wang

et al. (2010a). Since all functional brain areas are correlated, the matrix W has the structure of the adjacency matrix A_{K_N} of the complete graph K_N, where the one elements a_{ij} are substituted by the correlations $|w_{ij}| \leq 1$. Since the matrix norm $\|W\|_q \leq \|A_{K_N}\|_q$ because all elements $|w_{ij}| \leq 1$, **art.** 166 indicates that $\lambda_1 (W) \leq \|W\|_q$ and $\lambda_1 (W) \leq \lambda_1 (A_{K_N}) = N - 1$. Fig. 7.4 shows the eigenvalues of the weighted adjacency matrix W of the functional brain network of a typical patient before and after surgery. The correlations w_{ij} before and after surgery are almost the same. The spectrum in Fig. 7.4 is closely related to that of the complete graph K_N: the $\lambda_N = -1$ eigenvalue with multiplicity $N - 1$ in K_N is here spread over the interval $[-1, \lambda_1)$. All eigenvalues are simple and the largest eigenvalue in $[14, 15]$ is clearly most sensitivity to the changes in the weighted adjacency matrix W, as the insert in Fig. 7.4 shows. Hence, the changes in the few largest eigenvalues seem to be good indicators to evaluate the effect of the brain surgery.

The (weighted) adjacency matrix of any graph has at least two different eigen values as follows from **art.** 25. The complete graph is the only graph with $N > 2$ nodes that has precisely two different eigenvalues. Strongly regular graphs (**art.** 42) have three different eigenvalues. A small number of different eigenvalues implies a small diameter (**art.** 39). The weighted, symmetric adjacency matrix $W = W^T$ deviates from the zero one matrix and, with high probability, all of its eigenvalues are simple given that almost all real w_{ij} are different (**art.** 181).

7.4 Rewiring Watts-Strogatz small-world graphs

The spectrum of the Watts Strogatz small world graph G_{SWk} without link rewiring is computed in Section 5.2. Recall that G_{SWk} is a regular graph (**art.** 41) where each node has degree $r = 2k$. When links in G_{SWk} are rewired, independently and with probability p_r, the graph's topology and properties change with p_r. Fig. 1.3 presents a rewired Watts Strogatz small world graph, while the original regular small world graph G_{SWk} is shown in Fig. 5.1. Here, we investigate the influence of the link rewiring probability p_r on the eigenvalues of the adjacency matrix of Watts Strogatz small world graphs.

Fig. 7.5 shows the pdf $f_\lambda (x)$ of an eigenvalue λ of the adjacency matrix of a Watts Strogatz small world graph. In absence of randomness $p_r = 0$, the spectrum is discrete, reflected by the peaks in Fig. 7.5 and drawn differently for all k in Fig. 5.2. When randomness is introduced by increasing $p_r > 0$, the peaks smooth out and Fig. 7.5 indicates that the pdf $f_\lambda (x)$ tends rapidly to that of the Erdős Rényi random graph shown in Fig. 6.2.

Fig. 7.5 thus suggests that a bell shape of the spectrum around the origin is a fingerprint of "randomness" in a graph, while peaks reflect "regularity" or "struc ture"[1]. We also observe that "irregularity" can be measured, as mentioned in **art.** 43, by the amount that the largest eigenvalue deviates from the mean degree

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[1] The quotes here refer to an intuitive meaning. A commonly agreed and precise definition of "randomness" and "structure" of a graph is lacking.
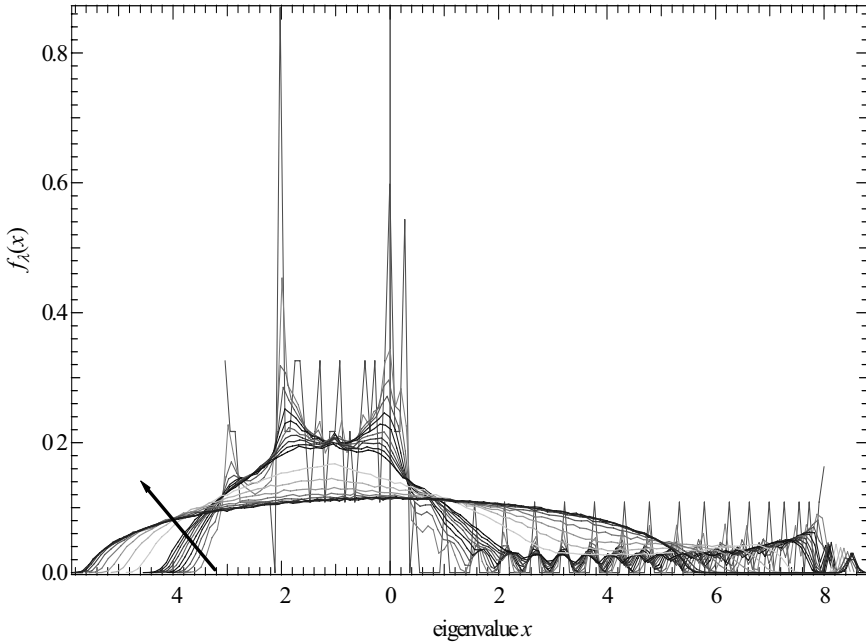
Fig. 7.5. The probability density function $f_\lambda(x)$ of an eigenvalue in Watts Strogatz small world graphs with $N = 200$ and $k = 4$ for various rewiring probabilities p_r ranging from 0 to 1, first in steps of 0.01 until $p_r = 0.1$, followed by an increase in steps of 0.1 up to $p_r = 1$. The arrow shows the direction of increasing p_r.

$E[D] = 2k$. Rewiring does not change the mean degree (because the number of links and nodes is kept constant and $E[D] = \frac{2L}{N}$), but we clearly see an increase of the largest eigenvalue from $\lambda_1 = 8 = 2k$ when $p_r = 0$ to about 9 for $p_r = 1$.

Fig. 5.3 has shown how irregular the number of different eigenvalues of $G_{\mathrm{SW}k}$ without rewiring behaves as a function of N and k. Simulations indicate that, even for a small rewiring probability of $p_r = 0.01$, the spectrum only contains simple eigenvalues with high probability. More precisely, when rewiring only one link in $G_{\mathrm{SW}k}$ with $N = 200$ and $k = 4$, the number of distinct eigenvalues dramatically increases from 95 to about 190. In other words, destroying the regular adjacency matrix structure by even one element has a profound impact on the multiplicity of the eigenvalues. This very high sensitivity is a known fact in the study of zeros of polynomials (Wilkinson, 1965, Chapter 2): small perturbations of the coefficients of a polynomial may heavily impact the multiplicity of the real zeros (and whether the perturbed zeros are still real).

Another consequence is that the upper bound in Theorem 5 on the diameter ρ in terms of the number of different eigenvalues is almost useless in real world graphs, where most of the eigenvalues are different, such that the bound in Theorem 5 re duces to $\rho \leq N-1 = \rho_{\max}$. By rewiring links in $G_{\mathrm{SW}k}$, we observe even contrasting

effects: the regular structure of G_{SWk} is destroyed, which causes the diameter, in most cases, to shrink, while the number of different eigenvalues suddenly jumps to almost the maximum N.

7.5 Assortativity

7.5.1 Theory

"Mixing" in complex networks refers to the tendency of network nodes to connect preferentially to other nodes with either similar or opposite properties. Mixing is computed via the correlations between the properties, such as the degree, of nodes in a network. Here, we study the degree mixing in undirected graphs. Generally, the linear correlation coefficient between two random variables of X and Y is defined (Van Mieghem, 2006b, p. 30) as

$$\rho(X, Y) = \frac{E[XY] - \mu_X \mu_Y}{\sigma_X \sigma_Y} \tag{7.1}$$

where $\mu_X = E[X]$ and $\sigma_X = \sqrt{\text{Var}[X]}$ are the mean and standard deviation of the random variable X, respectively. Newman (2003a, eq. (21)) has expressed the linear degree correlation coefficient of a graph as

$$\rho_D = \frac{\sum_{xy} xy (e_{xy} - a_x b_y)}{\sigma_a \sigma_b} \tag{7.2}$$

where e_{xy} is the fraction of all links that connect the nodes with degree x and y and where a_x and b_y are the fraction of links that start and end at nodes with degree x and y, satisfying the following three conditions:

$$\sum_{xy} e_{xy} = 1, \ a_x = \sum_y e_{xy} \text{ and } b_y = \sum_x e_{xy}$$

When $\rho_D > 0$, the graph possesses *assortative* mixing, a preference of high degree nodes to connect to other high degree nodes and, when $\rho_D < 0$, the graph features *disassortative* mixing, where high degree nodes are connected to low degree nodes.

The translation of (7.2) into the notation of random variables is presented as follows. Denote by D_i and D_j the node degree of two *connected* nodes i and j in an undirected graph with N nodes. In fact, we are interested in the degree of nodes at both sides of a link, without taking the link, that we are looking at, into consideration. As Newman (2003a) points out, we need to consider the number of excess links at both sides, and, hence the degree $D_{l^+} = D_i - 1$ and $D_{l^-} = D_j - 1$, where the link l has a start at $l^+ = i$ and an end at $l^- = j$. The linear correlation

coefficient of those excess degrees is

$$\rho\left(D_{l+}, D_{l^-}\right) = \frac{E\left[D_{l+}D_{l^-}\right] - E\left[D_{l+}\right]E\left[D_{l^-}\right]}{\sigma_{D_{l+}}\sigma_{D_{l^-}}}$$

$$= \frac{E\left[\left(D_{l+} - E\left[D_{l+}\right]\right)\left(D_{l^-} - E\left[D_{l^-}\right]\right)\right]}{\sqrt{E\left[\left(D_{l+} - E\left[D_{l+}\right]\right)^2\right]E\left[\left(D_{l^-} - E\left[D_{l^-}\right]\right)^2\right]}}$$

Since $D_{l+} - E\left[D_{l+}\right] = D_i - E\left[D_i\right]$, subtracting one link everywhere does not change the linear correlation coefficient, provided $D_i > 0$ (and similarly that $D_j > 0$), which is the case if there are no isolated nodes. Removing isolated nodes from the graph does not alter the linear degree correlation coefficient (7.2). Hence, we can assume that the graph has no zero degree nodes. In summary, the linear degree correlation coefficient is

$$\rho\left(D_{l+}, D_{l^-}\right) = \rho\left(D_i, D_j\right) = \frac{E\left[D_i D_j\right] - \mu_{D_i}^2}{E\left[D_i^2\right] - \mu_{D_i}^2} \tag{7.3}$$

We now proceed by expressing $E\left[D_i D_j\right]$, $E\left[D_i\right]$ and σ_{D_i} in the definition of $\rho\left(D_{l+}, D_{l^-}\right) = \rho\left(D_i, D_j\right)$ for undirected graphs in terms of more appropriate quantities of algebraic graph theory. First, we have that

$$E\left[D_i D_j\right] = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N}d_i d_j a_{ij} = \frac{d^T A d}{2L}$$

where d_i and d_j are the elements in the degree vector $d = (d_1, d_2, ..., d_N)$, and a_{ij} is the element (1.1) of the (symmetric) adjacency matrix A, that expresses connectivity between node i and j. The quadratic form $d^T A d$ can be written in terms of the total number $N_k = u^T A^k u$ of walks with k hops (**art.** 33). The total number $N_3 = d^T A d$ of walks with three hops is called the s metric in Li *et al.* (2006). The average μ_{D_i} and μ_{D_j} are the mean node degree of the two connected nodes i and j, respectively, and not the mean of the degree D of a random node, which equals $E\left[D\right] = \frac{2L}{N}$. Thus,

$$\mu_{D_i} = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N}d_i a_{ij} = \frac{1}{2L}\sum_{i=1}^{N}d_i\sum_{j=1}^{N}a_{ij} = \frac{1}{2L}\sum_{i=1}^{N}d_i^2 = \frac{d^T d}{2L}$$

while

$$\mu_{D_j} = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N}d_j a_{ij} = \mu_{D_i}$$

The variance $\sigma_{D_i}^2 = \text{Var}[D_i] = E\left[D_i^2\right] - \mu_{D_i}^2$ and

$$E\left[D_i^2\right] = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N}d_i^2 a_{ij} = \frac{1}{2L}\sum_{i=1}^{N}d_i^3 = E\left[D_j^2\right]$$

After substituting all terms into the expression (7.3) of the linear degree correlation

coefficient, we obtain, with $N_1 = 2L$ and $N_2 = d^T d$, our reformulation of Newman's definition (7.2) in terms of N_k,

$$\rho_D = \rho(D_i, D_j) = \frac{N_1 N_3 - N_2^2}{N_1 \sum\limits_{i=1}^{N} d_i^3 - N_2^2} \tag{7.4}$$

The crucial understanding of (dis)assortativity lies in the total number N_3 of walks with three hops compared to those with two hops, N_2, and one hop, $N_1 = 2L$.

7.5.1.1 Discussion of (7.4)

As shown in **art. 35**, the total number $N_k = u^T A^k u$ of walks of length k is upper bounded by

$$N_k \leq \sum_{j=1}^{N} d_j^k$$

with equality only if $k \leq 2$ and, for all k, only if the graph is regular. Hence, (7.4) shows that only if the graph is regular, $\rho_D = 1$, implying that maximum assortativity is only possible in regular graphs[2]. Since the variance of the degrees at one side of an arbitrary link

$$\sigma_{D_i}^2 = \frac{1}{N_1} \sum_{i=1}^{N} d_i^3 - \left(\frac{N_2}{N_1} \right)^2 \geq 0 \tag{7.5}$$

the sign of $N_1 N_3 - N_2^2$ in (7.4) distinguishes between assortativity ($\rho_D > 0$) and disassortativity ($\rho_D < 0$). The sign of $N_1 N_3 - N_2^2$ can also be determined from (4.58). Using (3.23) and denoting a link $l = i \sim j$, the degree correlation (7.4) can be rewritten as

$$\rho_D = 1 - \frac{\sum_{i \sim j} (d_i - d_j)^2}{\sum\limits_{i=1}^{N} d_i^3 - \frac{1}{2L} \left(\sum\limits_{i=1}^{N} d_i^2 \right)^2} \tag{7.6}$$

The graph is zero assortative ($\rho_D = 0$) if

$$N_2^2 = N_1 N_3 \tag{7.7}$$

We can show that the connected Erdős Rényi random graph $G_p(N)$ is zero assortative for all N and link density $p = L/\binom{N}{2} > p_c$, where p_c is the disconnectivity threshold. Asymptotically for large N, the Barabási Albert power law graph is zero assortative as shown in Nikoloski *et al.* (2005).

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[2] Notice that the definition (7.4) is inadequate (due to a zero denominator and numerator) for a regular graph with degree r because $N_{k \text{ regular graph}} \quad N r^k$ (**art.** 33). For regular graphs where $\sum_{i=1}^{N} d_i^3 \quad N_3$, the perfect disassortativity condition (7.8) becomes $N_2^2 \quad N_1 N_3$, which is equal to the zero assortativity condition (7.7). One may argue that $\rho_{D;\text{regular graph}} \quad 1$, since all degrees are equal and thus perfectly correlated. On the other hand, the complete graph K_N minus one link l has $\rho_D(K_N \backslash \{l\}) \quad \frac{-2}{N-1}$, which suggests that $\rho_D(K_N) \quad 0$ instead of 1.

Perfect disassortativity ($\rho_D = -1$ in (7.4)) implies that

$$N_2^2 = \frac{N_1}{2}\left(N_3 + \sum_{i=1}^{N} d_i^3\right) \tag{7.8}$$

For a complete bipartite graph $K_{m,n}$ (Section 5.7), we have that

$$\sum_{i \sim j}(d_i - d_j)^2 = mn\,(n-m)^2,\ \sum_{i=1}^{N}d_i^3 = nm\,(n^2 + m^2)\ \text{and}\ \sum_{i=1}^{N}d_i^2 = nm\,(n+m)$$

such that (7.6) becomes $\rho_D = -1$, provided $m \neq n$. Hence, any complete bipartite graph $K_{m,n}$ (irrespective of its size and structure (m, n), except for the regular graph variant where $m = n$) is perfectly disassortative. The perfect disassortativity of complete bipartite graphs is in line with the definition of disassortativity, because each node has only links to nodes of a different set with different properties. Nevertheless, the fact that all complete bipartite graphs $K_{m,n}$ with $m \neq n$ have $\rho_D = -1$, even those with nearly the same degrees $m = n \pm 1$ and thus close to regular graphs typified by $\rho_D = 1$, shows that assortativity and disassortativity of a graph is not easy to predict. It remains to be shown that the complete bipartite graphs $K_{m,n}$ with $m \neq n$ are the only perfect disassortative class of graphs.

There is an interesting relation between the linear degree correlation coefficient ρ_D of the graph G and the variance of the degree of a node in the corresponding line graph $l\,(G)$ (**art. 7**). The l th component of the $L \times 1$ degree vector in the line graph $l\,(G)$ (**art. 8**) is $\left(d_{l(G)}\right)_l = d_i + d_j - 2$, where node i and node j are connected by link $l = i \sim j$. The variance of the degree $D_{l(G)}$ of a random node in the line graph equals

$$\text{Var}\left[D_{l(G)}\right] = E\left[(D_i + D_j)^2\right] - (E\,[D_i + D_j])^2$$

which we rewrite as

$$\text{Var}\left[D_{l(G)}\right] = 2\left(E\left[D_i^2\right] - \mu_{D_i}^2 + E\,[D_i D_j] - \mu_{D_i}^2\right)$$

Using (7.3), we arrive at

$$\text{Var}\left[D_{l(G)}\right] = 2\,(1 + \rho_D)\left(E\left[D_i^2\right] - \mu_{D_i}^2\right) = 2\,(1 + \rho_D)\,\text{Var}\,[D_i]$$

$$= 2\,(1 + \rho_D)\left(\frac{1}{N_1}\sum_{i=1}^{N}d_i^3 - \left(\frac{N_2}{N_1}\right)^2\right) \tag{7.9}$$

Curiously, the expression (7.9) shows for perfect disassortative graphs ($\rho_D = -1$) that $\text{Var}\left[D_{l(G)}\right] = 0$. The latter means that $l\,(G)$ is then a regular graph, but this does not imply that the original graph G is regular. Indeed, if G is regular, then $l\,(G)$ is also regular as follows from the l th component of the degree vector, $\left(d_{l(G)}\right)_l = d_i + d_j - 2$. However, the reverse is not necessarily true: it is possible that $l\,(G)$ is regular, while G is not, as shown above, for complete bipartite graphs $K_{m,n}$ with $m \neq n$ that are not regular. In summary, in both extreme cases $\rho_D = -1$ and $\rho_D = 1$, the corresponding line graph $l\,(G)$ is a regular graph.

7.5.1.2 Relation between λ_1 and ρ_D

The largest eigenvalue λ_1 of the adjacency matrix A of a graph is an important characterizer of a graph. Here, we present a new lower bound for λ_1 in terms of the linear degree correlation coefficient ρ_D. **Art.** 44 presents improvements on the classical lower bound (3.31) for λ_1 in terms of N_k. For $k = 3$ in (3.33) and using (7.4), we obtain

$$\lambda_1^3 \geq \frac{N_3}{N} = \frac{1}{N}\left(\rho_D\left(\sum_{i=1}^{N} d_i^3 - \frac{N_2^2}{N_1}\right) + \frac{N_2^2}{N_1}\right) \qquad (7.10)$$

This last inequality (7.10) with (7.5) shows that the lower bound for the largest eigenvalue λ_1 of the adjacency matrix A is strictly increasing in the linear degree correlation coefficient ρ_D (except for regular graphs). Given the degree vector d is constant, inequality (7.10) shows that the largest eigenvalue λ_1 is obtained, in the case where we succeed in increasing the assortativity of the graph by degree preserving rewiring, which is discussed in Section 7.5.2.
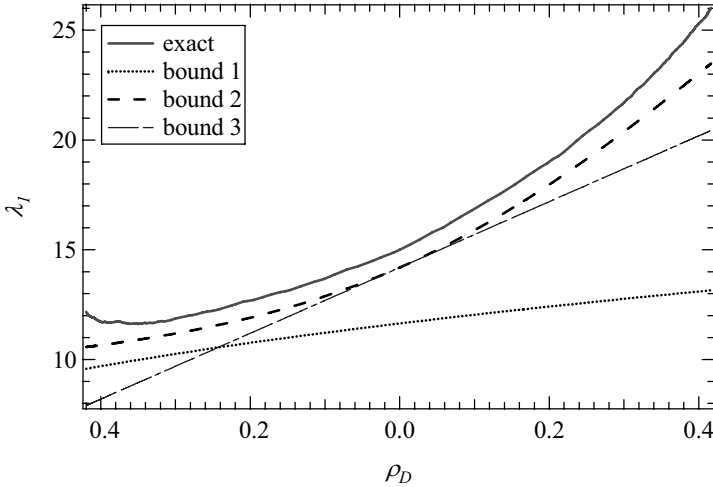
Fig. 7.6. The largest eigenvalue λ_1 of the Barabási Albert power law graph with $N = 500$ nodes and $L = 1960$ links versus the linear degree correlation coefficient ρ_D. Various lower bounds are plotted: bound 1 is (7.10), bound 2 is (3.40) and bound 3 is (3.35) for $m = 1$. The corresponding classical lower bound (3.31) is 7.84, while the lower bound (3.34) is 10.548. The latter two lower bounds are independent of ρ_D.

Fig. 7.6 illustrates how the largest eigenvalue λ_1 of the Barabási Albert power law graph evolves as a function of the linear degree correlation coefficient ρ_D, which can be changed by degree preserving rewiring. The lower bound (3.40) clearly outperforms the lower bound[3] (7.10).

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[3] Especially for strong negative ρ_D, we found   very rarely though   that (3.40) can be slightly worse than (3.34).

The Rayleigh principle in **art.** 88 provides an upper bound for the second smallest eigenvalue $\mu_{N\ 1}$ of the Laplacian Q for the choice $g(n) = d_n$, the degree of a node n,

$$\mu_{N\ 1} \leq \frac{\sum_{l \in \mathcal{L}} (d_{l+} - d_{l\ })^2}{\sum_{j=1}^{N} d_j^2 - \frac{1}{N} \left(\sum_{j=1}^{N} d_j \right)^2}$$

After introducing (7.6), we find for any non regular graph

$$\mu_{N\ 1} \leq (1 - \rho_D) \frac{\sum_{i=1}^{N} d_i^3 - \frac{1}{2L} \left(\sum_{i=1}^{N} d_i^2 \right)^2}{\sum_{j=1}^{N} d_j^2 - \frac{1}{N} \left(\sum_{j=1}^{N} d_j \right)^2} = (1 - \rho_D) \frac{E[D]\, E[D^3] - \left(E[D^2] \right)^2}{E[D]\, \mathrm{Var}[D]}$$

(7.11)

which is an upper bound for the algebraic connectivity $\mu_{N\ 1}$ in terms of the linear correlation coefficient of the degree ρ_D. In degree preserving rewiring, the fraction in (7.11), which is always positive, is unchanged and we observe that the upper bound decreases linearly in ρ_D.

7.5.2 Degree-preserving rewiring

In degree preserving rewiring, links in a graph are rewired while maintaining the degree distribution unchanged. This means that the degree vector d is constant and, consequently, that $N_1 = \sum_{i=1}^{N} d_i$, $N_2 = \sum_{i=1}^{N} d_i^2$ and $\sum_{i=1}^{N} d_i^3$ do not change during degree preserving rewiring, only N_3 does, and, by (7.4), also the (dis)assortativity ρ_D.

Degree preserving rewiring changes only the term $\sum_{i \sim j} (d_i - d_j)^2$ in (7.6), which allows us to understand how a degree preserving rewiring operation changes the linear degree correlation ρ_D. Each step in degree preserving random rewiring consists of first randomly selecting two links $i \sim j$ and $k \sim l$ associated with the four nodes i, j, k, l. Next, the links can be rewired either into $i \sim k$ and $j \sim l$ or into $i \sim l$ and $j \sim k$.

Theorem 35 *Given a graph in which two links are degree preservingly rewired. We order the degree of the four involved nodes as $d_{(1)} \geq d_{(2)} \geq d_{(3)} \geq d_{(4)}$. The two links are associated with the four nodes $n_{d_{(1)}}, n_{d_{(2)}}, n_{d_{(3)}}$ and $n_{d_{(4)}}$ only in one of the following three ways: (a) $n_{d_{(1)}} \sim n_{d_{(2)}}, n_{d_{(3)}} \sim n_{d_{(4)}}$, (b) $n_{d_{(1)}} \sim n_{d_{(3)}}, n_{d_{(2)}} \sim n_{d_{(4)}}$ and (c) $n_{d_{(1)}} \sim n_{d_{(4)}}, n_{d_{(2)}} \sim n_{d_{(3)}}$. The corresponding linear degree correlation introduced by these three possibilities obeys $\rho_a \geq \rho_b \geq \rho_c$.*

Proof: In these three ways of placing the two links, the degree of each node remains the same. According to the definition (7.6), the linear degree correlation

changes only via $\varepsilon = -\sum_{i \sim j} (d_i - d_j)^2$. Thus, the relative degree correlation difference between (a) and (b) is

$$\varepsilon_a - \varepsilon_b = -\left(d_{(1)} - d_{(2)}\right)^2 - \left(d_{(3)} - d_{(4)}\right)^2 + \left(d_{(1)} - d_{(3)}\right)^2 + \left(d_{(2)} - d_{(4)}\right)^2$$
$$= 2(d_{(2)} - d_{(3)})(d_{(1)} - d_{(4)}) \geq 0$$

since the rest of the graph remains the same in all three cases. Similarly,

$$\varepsilon_a - \varepsilon_c = 2(d_{(2)} - d_{(4)})(d_{(1)} - d_{(3)}) \geq 0$$
$$\varepsilon_b - \varepsilon_c = 2(d_{(1)} - d_{(2)})(d_{(3)} - d_{(4)}) \geq 0$$

These three inequalities prove the theorem. □

A direct consequence of Theorem 35 is that we can now design a rewiring rule that increases or decreases the linear degree correlation ρ_D of a graph. We define *degree preserving assortative rewiring* as follows: randomly select two links associated with four nodes and then rewire the two links such that as in (a) the two nodes with the highest degree and the two lowest degree nodes are connected. If any of the new links exists before rewiring, discard this step and a new pair of links is randomly selected. Similarly, the procedure for *degree preserving disassortative rewiring* is: randomly select two links associated with four nodes and then rewire the two links such that as in (c) the highest degree node and the minimum degree node are connected, while also the remaining two nodes are linked provided the new links do not exist before rewiring. Theorem 35 shows that the degree preserving assortative (disassortative) rewiring operations increase (decrease) the degree correlation of a graph.

The assortativity range, defined as difference $\max\rho_D - \min\rho_D$, may be regarded as a metric of a given degree vector d, which reflects its adaptivity in (dis)assortativity under degree preserving rewiring. As shown earlier, for some graphs such as regular graphs, that difference $\max\rho_D - \min\rho_D = 0$, while $\max\rho_D - \min\rho_D \leq 2$ because $-1 \leq \rho_D \leq 1$.

Degree preserving rewiring is an interesting tool to modify a graph in which the resources of the nodes are constrained. For instance, the number of outgoing links in a router as well as the number of flights per day at many airports are almost fixed.

As an example, we consider degree preserving rewiring in the US air transportation network[4], where each node is an American airport and each link is a flight connection between two airports. We are interested in an infection process, where viruses are spread via airplanes from one city to another. From a topological point of view, the infection threshold $\tau_c = \frac{1}{\lambda_1}$ is the critical design parameter, which we would like to have as high as possible because an effective infection rate $\tau > \tau_c$ translates into a certain percentage of people that remain infected after sufficiently long time (for details see Van Mieghem *et al.* (2009)). Since most airports operate near to full capacity, the number of flights per airport should hardly

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[4] The number of nodes is N ≈ 2179 and the number of links is L ≈ 31326.

Fig. 7.7. The ten largest and five smallest eigenvalue of the adjacency matrix of the USA airport transport network versus the percentage of rewired links. The insert shows the linear degree correlation coefficient ρ_D as a function of the assortative degree preserving rewiring.

change during the re engineering to modify the largest eigenvalue λ_1. Fig. 7.7 shows how the adjacency eigenvalues of the US air transportation network changes with degree preserving assortative rewiring, while the disassortive companion figure is also shown in Van Mieghem *et al.* (2010). In each step of the rewiring process, only four one elements (i.e., two links) in the adjacency matrix change position. If we relabel the nodes in such a way that the link between 1 and 2 and between 3 and 4 (case (a) in Theorem 35) is rewired to either case (b) or (c), then only a 4×4 submatrix A_4 of the adjacency matrix A in

$$A = \left[\begin{array}{cc} A_4 & C \\ C^T & A_c \end{array} \right]$$

is altered. The Interlacing Theorem 42 states that $\lambda_{j+4}(A) \leq \lambda_j(A_c) \leq \lambda_j(A)$ for $1 \leq j \leq N - 4$, which holds as well for A_r after just one degree preserving rewiring step. Thus, most of the eigenvalues of A and A_r are interlaced, as observed from Fig. 7.7. The large bulk of the 2179 eigenvalues (not shown in Fig. 7.7) remains cen tered around zero and confined to the almost constant white strip between λ_{10} and λ_N 5. As shown in Section 7.5.1.2, assortative rewiring increases λ_1. Fig. 7.7 illus trates, in addition, that the spectral width or range $\lambda_1 - \lambda_N$ increases as well, while the spectral gap $\lambda_1 - \lambda_2$ remains high, in spite of the fact that the algebraic connec tivity μ_N 1 is small. In fact, Fig. 7.8 shows that μ_N 1 decreases, in agreement with
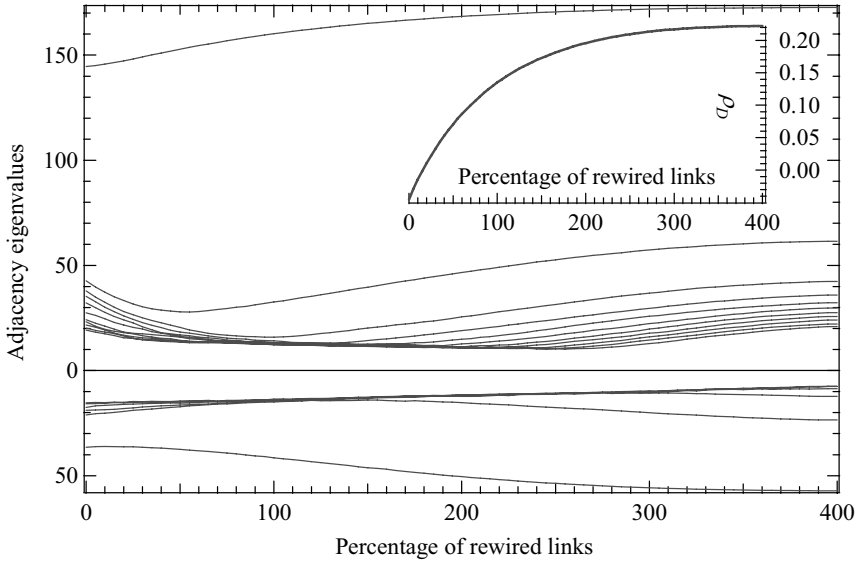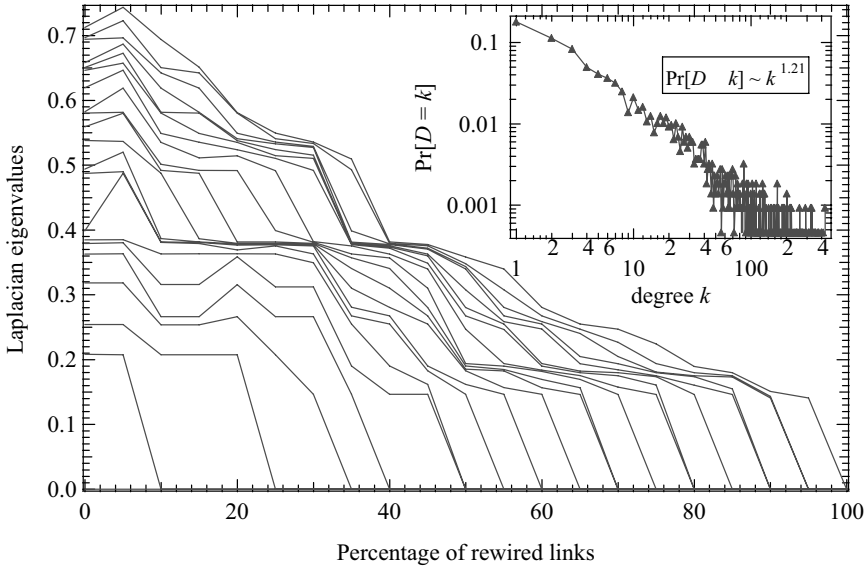
Fig. 7.8. The twenty smallest eigenvalues of the Laplacian matrix of the US air trans
portation network versus the percentage of rewired links. The insert shows the degree
distribution that is maintained in each degree preserving rewiring step.

(7.11), and vanishes after about 10% of the link rewirings, which indicates (**art.** 80)
that the graph is then disconnected. Fig. 7.8 further shows that by rewiring all links
on average once (100%), assortative degree preserved rewiring has dissected the US
air transportation network into 20 disconnected clusters. Increasing assortativity
implies that high degree and low degree nodes are linked increasingly more to each
other, which, intuitively, explains why disconnectivity in more and more clusters
start occurring during the rewiring process.

The opposite occurs in disassortative rewiring: the algebraic connectivity μ_{N-1}
was found to increase during degree preserving rewiring from about 0.25 to almost 1,
which is the maximum possible due to (4.23) and $d_{\min} = 1$ as follows from the insert
in Fig. 7.8. Hence, in order to suppress virus propagation via air transport while
guaranteeing connectivity, disassortative degree preserving rewiring is advocated,
which, in return, enhances the topological robustness as explained in **art.** 97.

Finally, we mention that highly disassortative graphs possess a zero eigenvalue of
the adjacency matrix with large multiplicity, which can be understood from Section
7.1.1: high degree nodes are preferentially connected to a large set of low degree
nodes, that are not interconnected among themselves.

7.6 Reconstructability of complex networks

In this section, we investigate, given the set of eigenvectors $x_1, x_2, \ldots, x_N$, how many eigenvalues of the adjacency matrix A are needed to be able to reconstruct A exactly. Specifically, we perturb the spectrum by omitting the j smallest eigenvalues in absolute value of A and we determine the maximal value of j such that the matrix A can be exactly reconstructed.

Since $\sum_{j=0}^{N} \lambda_j = 0$ (**art. 25**), on average half of the eigenvalues of the adjacency matrix A are negative. Therefore, we reorder the eigenvalues as $\left|\lambda_{(1)}\right| \leq \left|\lambda_{(2)}\right| \leq \cdots \leq \left|\lambda_{(N)}\right|$ such that $\lambda_{(j)}$ is the j th smallest (in absolute value) eigenvalue corre sponding to the eigenvector $x_{(j)}$. Let us define the $N \times N$ matrices

$$\Lambda_{(j)} = \mathrm{diag}\left(0, \ldots, 0, \lambda_{(j+1)}, \lambda_{(j+2)}, \cdots, \lambda_{(N)}\right)$$

and

$$A_{(j)} = \tilde{X}\Lambda_{(j)}\tilde{X}^T$$

where $\tilde{X} = \begin{bmatrix} x_{(1)} & x_{(2)} & \cdots & x_{(N)} \end{bmatrix}$ is the reordered version of the orthogonal matrix X in (1.2) corresponding to the eigenvalues ranked in absolute value. Thus, $\Lambda_{(j)}$ is the diagonal matrix where the j smallest (in absolute value) eigenvalues are put equal to zero, or, equivalently, are removed from the spectrum of A. The spectral perturbation here considered consists of consecutively removing more eigen values from the spectrum until we can no longer reconstruct the adjacency matrix A. Clearly, when $j = 0$, we have that $A_{(0)} = A$ and that, for any other $j > 0$, $A_{(j)} \neq A$. Moreover, when $j > 0$, $A_{(j)}$ is not a zero one matrix anymore. Fig. 7.9 plots the histograms of the entries of $A_{(5)}$, $A_{(10)}$, $A_{(15)}$ and $A_{(20)}$ for an Erdős Rényi random graph with $N = 36$ nodes and link density of $p = 0.5$. The removal of a part of the eigenvalues causes roughly the same impact on the 1 and 0 elements of the adjacency matrix A, as shown in Fig. 7.9. This means that the deviations on 1s and 0s are almost the same, and that the distribution of values around 1 and 0 will reach $1/2$ roughly simultaneously, when the number of removed eigenvalues increases gradually. Using Heavyside's step function $h(x)$,

$$h(x) = \begin{cases} 0 & \text{if } x < 0 \\ \frac{1}{2} & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

we truncate the elements of $A_{(j)}$ as $h\left(\left(A_{(j)}\right)_{ij} - \frac{1}{2}\right)$. If we now define the operator $\mathcal{H}$ applied to a matrix $A_{(j)}$ that replaces each element of $A_{(j)}$ by $h\left(\left(A_{(j)}\right)_{ij} - \frac{1}{2}\right)$, then

$$\widetilde{A_j} = \mathcal{H}\left(A_{(j)}\right)$$

is a zero one matrix, with the possible exception of elements $\frac{1}{2}$. The interesting observation from extensive simulation is that there seems to exist a maximal number
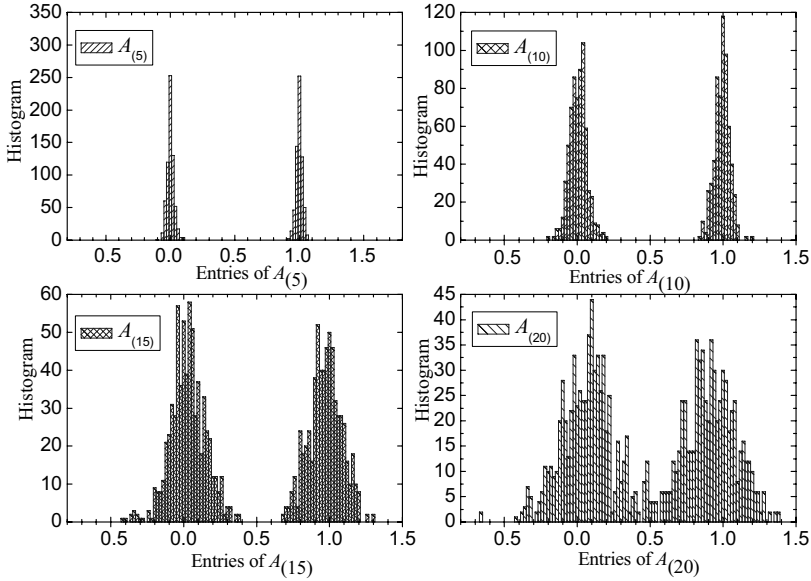
Fig. 7.9. The histograms of the entries of $A_{(5)}$, $A_{(10)}$, $A_{(15)}$ and $A_{(20)}$. The matrix A ($A = A_{(0)}$) is the adjacency matrix of an Erdős Rényi random graph with $N = 36$ nodes and link density $p = 0.5$.

θ, such that

$$\widetilde{A_j} = A, \text{ if } j \leq \theta$$
$$\widetilde{A_j} \neq A, \text{ if } j > \theta$$

In other words, θ is the maximum number of eigenvalues that can be removed from the spectrum of the graph such that the graph can still be reconstructed precisely, given the matrix X. We therefore call θ the *reconstructability coefficient*.

7.6.1 Theory

Art. 156 shows that any real, symmetric matrix A can be rewritten as (8.31),

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

where the matrix $E_k = x_k x_k^T$ is the outer product of x_k by itself. Any element of A can be written, with the above relabelling of the eigenvectors according to a

ranking in absolute values of the eigenvalues $\left|\lambda_{(1)}\right| \leq \left|\lambda_{(2)}\right| \leq \cdots \leq \left|\lambda_{(N)}\right|$ as

$$a_{ij} = \sum_{k=1}^{m} \lambda_{(k)} \left(E_{(k)}\right)_{ij} + \sum_{k=m+1}^{N} \lambda_{(k)} \left(E_{(k)}\right)_{ij} \tag{7.12}$$

where $m \in [1, N]$ is, for the time being, an integer. As shown in **art. 157**, the 2 norm of E_k is not larger than 1, so that $\left|\left(E_{(k)}\right)_{ij}\right| \leq 1$ for any $1 \leq k \leq N$, which implies that $-1 \leq \left(E_{(k)}\right)_{ij} \leq 1$. Relation (8.31) also explains why an ordering in absolute value is most appropriate for our spectral perturbation: the usual ordering $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N\,_1 \geq \lambda_N$ in algebraic graph theory would first remove $\lambda_N < 0$, then $\lambda_N\,_1$ and so on. However, $|\lambda_N|$ can be large and its omission from the spectrum is likely to cause too big an impact.

The reconstructability of a graph is now reformulated as follows. Since a_{ij} is either zero or one, it follows from (7.12) that, if

$$\left|a_{ij} - \sum_{k=m+1}^{N} \lambda_{(k)} \left(E_{(k)}\right)_{ij}\right| < \frac{1}{2} \tag{7.13}$$

we can reconstruct the element a_{ij} as

$$a_{ij} = \begin{cases} 1 & \text{if } \sum_{k=m+1}^{N} \lambda_{(k)} \left(E_{(k)}\right)_{ij} > \frac{1}{2} \\ 0 & \text{if } \sum_{k=m+1}^{N} \lambda_{(k)} \left(E_{(k)}\right)_{ij} < \frac{1}{2} \end{cases}$$

The reconstructability requirement (7.13) determines the values of m that satisfy the inequality. The largest value of m obeying (7.13) is denoted by θ, called the reconstructability coefficient of a graph.

Using (7.12), the reconstructability requirement (7.13) is equivalent to

$$\left|\sum_{k=1}^{\theta} \lambda_{(k)} \left(E_{(k)}\right)_{ij}\right| < \frac{1}{2}$$

A further analysis is difficult due to the appearance of the matrix elements $\left(E_{(k)}\right)_{ij}$, of which, in general, not much is known. Since $\left|\left(E_{(k)}\right)_{ij}\right| \leq 1$, we can bound the sum as

$$\left|\sum_{k=1}^{\theta} \lambda_{(k)} \left(E_{(k)}\right)_{ij}\right| \leq \sum_{k=1}^{\theta} \left|\lambda_{(k)}\right| \left|\left(E_{(k)}\right)_{ij}\right| \leq \sum_{k=1}^{\theta} \left|\lambda_{(k)}\right| \tag{7.14}$$

In many cases, this bound is conservative because, on average, half of the eigenvalues of the adjacency matrix A is negative. Moreover, the matrix element $\left(E_{(k)}\right)_{ij}$ can also be negative. Liu *et al.* (2010) show for the class $G_p(N)$ of Erdős Rényi random graphs that the bound (7.14) is, indeed, too conservative and that only extensive simulations seem appropriate to determine the reconstructability coefficient θ.

7.6.2 The average the reconstructability coefficient $E[\theta]$

Via extensive simulations, Liu *et al.* (2010) investigated the properties of the re constructability coefficient θ for several important types of complex networks intro duced in Section 1.3, such as Erdős Rényi random graphs, Barabási Albert scale free networks and Watts Strogatz small world networks, and also other special de terministic types of graphs. A general linear scaling law was found:

$$E[\theta] = aN \qquad (7.15)$$

where the real number $a \in [0,1]$ depends on the graph G. Moreover, the variance $\mathrm{Var}[\theta]$ was sufficiently smaller than the mean $E[\theta]$ such that $E[\theta]$ serves as an excel lent estimate for θ. For sufficiently large N, a portion a of the smallest eigenvalues (in absolute value) can be removed from the spectrum and the adjacency matrix is still reconstructable with its original eigenvectors. The magnitude of a for different types of complex networks with different parameters was found to vary from 39% to 76%, which is surprisingly high.

The basic eigenvalue relation (8.31) shows that the set of orthogonal eigenvec tors are weighted by their corresponding eigenvalues. Any eigenvector specifies an orthogonal direction in the N dimensional space (see Section 1.1). The eigenvector with an eigenvalue in absolute value close to zero contains redundant information about the topology of the graph, in the sense that after the removal of this eigen value the network can still be reconstructed from the remaining spectrum. Liu *et al.* (2010) observe that when the graphs are more "regularly structured", the parame ter a seems higher. Deterministic graphs, like path, ring and lattice graphs, are more "regularly structured" than Erdős Rényi random graphs, power law graphs and rewired small world graphs. In the spectral domain, the more regular a graph is, the more constraints it needs to obey, and the less the N dimensional space is "sampled". In other words, the fewer the number spectral bases (eigenvectors) that are needed to reconstruct the graph. One may also say that the embedding of the graph structure in the N dimensional space does not need those orthogonal dimensions (which act similarly as a kernel of a linear transformation).

The reconstructability coefficient θ (or the scaled one coefficient $a = \frac{E[\theta]}{N}$ in (7.15)) can be regarded as a spectral metric of the graph that expresses how many dimensions of the N dimensional space are needed to represent or reconstruct the graph. Roughly, a high reconstructability coefficient θ reflects a "geometrically simple" graph that only needs a few orthogonal dimensions to be described. The precise physical or topological meaning of the reconstructability coefficient θ is not yet entirely clear. Finally, it would be desirable to have a rigorous proof of the claimed linear law (7.15).

7.7 Reaching consensus

Each node j in a network possesses a value $x_j[0]$ at discrete time $k = 0$. That value can be an estimate of, for example, the temperature, the pressure, the traffic

load, measured by each sensor node in the network, or it can represent an opinion score in a social network. The goal is to reach consensus among all the nodes in the network about the value x over time. All nodes exchange their value with their neighbors at discrete time k and they update their value at time $k + 1$. A simple updating strategy is a weighted sum,

$$x_j [k + 1] = w_{jj} [k] x_j [k] + \sum_{l \text{ is a neighbor of } j} w_{lj} [k] x_j [k]$$

where $w_{lj} [k]$ is the weight that node j applies at time k to the value received from the neighboring node l. Given the initial vector $x [0]$, the governing equations for the dynamic consensus process are, in matrix form,

$$x [k + 1] = W [k] x [k]$$

where we can consider $W [k]$ as a weighted adjacency matrix at time k plus a diagonal matrix $\text{diag} \left(\{ w_{jj} \}_{1 \leq j \leq N} \right)$, because $a_{jj} = 0$ and, here, the diagonal values are usually the most important ones. The formal solution is obtained by iteration as

$$x [k] = W [k - 1] W [k - 2] \ldots W [0] x [0]$$

This matrix equation is similar to the system equation of a Markov process, where $W [k]$ is then the stochastic transition probability matrix at time k. Section 3.7 describes the time convergence of a random walk on a graph towards the steady state.

A simple example of this linear updating strategy is

$$W [k] = I - wQ [k] = I - w\Delta [k] + wA [k]$$

where w is chosen such that $W [k]$ is a non negative, symmetric matrix and that consensus is reached rapidly. The whole dynamics of the process then depends on the time dependence of the graph, reflected by the corresponding Laplacian $Q [k]$. A further simplification lies in considering a static weight matrix $W [k] = W$. The consensus dynamically behaves in that case as

$$x [k] = W^k x [0] = (I - wQ)^k x [0]$$

which is entirely determined by the eigenvalues and eigenvectors of the matrix $I - wQ$. The eigenvalues $\{ \xi_j \}_{1 \leq j \leq N}$ of $I - wQ$ are equal to the set $\{ 1 - w\mu_j \}_{1 \leq j \leq N}$ with corresponding eigenvectors equal to those of the Laplacian Q. Fast convergence and non negativity requires that each eigenvalue of $I - wQ$ obeys $0 \leq \xi_j \leq 1$, which implies with (4.10) that $w < \frac{1}{\mu_1}$ or, safely, $w < \frac{1}{2d_{\max}}$.

7.8 Spectral graph metrics

Most of the graph metrics, such as the hopcount, diameter, clustering coefficient, and many more listed in Section 1.4, are defined in the topology domain. In this

section, we deal with graph metrics that are defined in the spectral domain. We have already encountered some spectral graph metrics such as the algebraic connectivity $\mu_{N\ 1}$ in Section 4.2 and the reconstructability coefficient θ in Section 7.6.

7.8.1 Eigenvector centrality

The per component eigenvalue equation (1.3) of the k th eigenvector,

$$(x_k)_j = \frac{(Ax_k)_j}{\lambda_k} = \frac{1}{\lambda_k} \sum_{l \text{ is a direct neighbor of } j} (x_k)_l \tag{7.16}$$

is called the eigenvector centrality of node j according to the eigenvector x_k of the adjacency matrix A of a graph G. This "centrality" measure reflects the importance with respect to the eigenvector x_k of a node in a network and provides a ranking of the nodes in the network according to the eigenvector x_k. Since the eigenvector x_1 has non zero components (**art.** 21), this largest eigenvector is considered most often. Perhaps the best known example of this spectral graph metric is Google's Page Rank, explained in Van Mieghem (2006b, Section 11.6), where the importance of webpages are ranked according to the components of the largest eigenvector of a weighted adjacency matrix, actually the stochastic matrix $P = \Delta^{-1}A$ of the web.

Since the eigenvectors of the symmetric adjacency matrix A are assumed to be orthogonal and normalized (**art.** 151), it holds that $-1 \le (x_k)_j \le 1$. Thus, the definition of eigenvector centrality (7.16) shows that

$$(x_k)_j \le \frac{1}{\lambda_k} \sum_{l \text{ is a direct neighbor of } j} 1 = \frac{d_j}{\lambda_k}$$

which suggests the interpretation of the eigenvector centrality (7.16) as a "weighted degree". Using (2.4), $d_j = (Au)_j$, **art.** 41 indicates that the eigenvector centrality of regular graphs, according to the largest eigenvalue, equals $(x_1)_j = \frac{1}{\sqrt{N}}$, which is constant for all nodes in the regular graph. Thus, for regular graphs, the eigenvector centrality is, essentially other than a scaling constant, the same as the degree.

7.8.2 Graph energy

The graph energy E_G is defined as

$$E_G = \sum_{j=1}^{N} |\lambda_j(A)| \tag{7.17}$$

The definition (7.17) of the graph energy is inspired by the energy eigenstates of the Hamiltonian applied to molecules (such as hydrocarbons) and was first proposed by Gutman (Dehmer and Emmert Streib, 2009, Chapter 7). The chemical origin does not directly help to interpret the notion of graph energy, so that the graph energy is best considered as one of the spectral metrics of a graph.

The absolute sign in the definition (7.17) complicates exact computations, but a large number of bounds exist. A direct application of the inequality (9.49) and **art.** 144 gives

$$(E_G - \lambda_1(A))^{2m} \leq (N-1)^{2m-1} \left\{ \text{trace}\left(A^{2m}\right) - \lambda_1^{2m}(A) \right\}$$

Rewritten with definition of $W_k = \text{trace}(A^k)$ in **art. 36**, we obtain, for any integer $m > 0$, the upper bound

$$E_G \leq \lambda_1(A) + (N-1)^{1-1/(2m)} \sqrt[2m]{W_{2m} - \lambda_1^{2m}(A)}$$

Since the function $f(x) = x + (N-1)^{1-1/(2m)} \sqrt[2m]{W_{2m} - x^{2m}}$ is decreasing in the interval $\arg_x \max f(x) \leq x \leq \sqrt[2m]{W_{2m}}$, a lower bound for $\lambda_1(A)$ of the type (3.33) with $k = 2m$ that lies in that interval can be used to derive a (slightly) less tight upper bound for E_G,

$$E_G \leq \sqrt[2m]{\frac{N_{2m}}{N}} + (N-1)^{1-1/(2m)} \sqrt[2m]{W_{2m} - \frac{N_{2m}}{N}}$$

For example, for $m = 1$, we obtain with (3.9)

$$E_G \leq \frac{2L}{N}\sqrt{1 + \frac{\text{Var}[D]}{(E[D])^2}} + \sqrt{(N-1)}\sqrt{2L - \left(\frac{2L}{N}\right)^2\left(1 + \frac{\text{Var}[D]}{(E[D])^2}\right)}$$

Other upper bounds are found in Dehmer and Emmert Streib (2009, Chapter 7). A lower bound is deduced from

$$E_G^2 = \sum_{j=1}^{N} \lambda_j^2(A) + \sum_{j=1}^{N}\sum_{k=1;k\neq j}^{N} |\lambda_j(A)|\,|\lambda_k(A)|$$

We apply the harmonic, geometric and arithmetic mean inequality (5.15) to the last sum

$$\frac{1}{N(N-1)}\sum_{j=1}^{N}\sum_{k=1;k\neq j}^{N} |\lambda_j(A)|\,|\lambda_k(A)| \geq \sqrt[N(N-1)]{\prod_{j=1}^{N}\prod_{k=1;k\neq j}^{N} |\lambda_j(A)|\,|\lambda_k(A)|}$$

With $\prod_{k=1}^{N} |\lambda_k(A)| = \left|\prod_{k=1}^{N} \lambda_k(A)\right| = |\det(A)|$ (**art. 138**), we have

$$\prod_{j=1}^{N}\prod_{k=1;k\neq j}^{N} |\lambda_j(A)|\,|\lambda_k(A)| = \prod_{j=1}^{N} |\lambda_j(A)|^{N-2}\prod_{k=1}^{N} |\lambda_k(A)| = \prod_{j=1}^{N} |\lambda_j(A)|^{N-2}|\det(A)|$$

$$= |\det(A)|^N \left(\prod_{j=1}^{N} |\lambda_j(A)|\right)^{N-2} = |\det(A)|^{2(N-1)}$$

such that with (3.2)

$$E_G \geq \sqrt{2L + N(N-1)\left(|\det(A)|\right)^{2/N}} = \sqrt{2}\sqrt{L + L_{\max}\left(|\det(A)|\right)^{2/N}}$$

Clearly, $E_G \geq \sqrt{2L}$.

The determination of graphs that maximize the graph energy E_G is an active domain of research. A complete solution is not known. We content ourselves here to list a few results and refer to Dehmer and Emmert Streib (2009, Chapter 7) for a detailed review of reported results. Obviously, the graph with minimum energy is the zero graph consisting of isolated nodes, i.e., the complement of the complete graph $(K_N)^c$. Among the trees, the star $K_{1,n}$ has minimal graph energy, whereas the path possesses maximum energy. A curiously observed fact from simulations, as mentioned by Gutman *et al.* in Dehmer and Emmert Streib (2009, Chapter 7), is that E_G seems to decrease almost linearly in the multiplicity of the zero eigenvalue for a certain class of graphs. Such an "almost[5]" linear scaling law bears resemblance to the linear scaling law (7.15) of the reconstructability coefficient.

7.8.3 Effective graph resistance

We consider a network in which a flow with magnitude I is injected in node a and the flow leaves the network at node b. As explained in Section 2.1.1, the in flows and out flows at a node i satisfy a conservation law:

$$\sum_{j \in \text{ neighbor}(i)} y_{ij} = \sum_{j=1}^{N} a_{ij}y_{ij} = I\left(1_{\{i=a\}} - 1_{\{i=b\}}\right) \tag{7.18}$$

where $y_{ij} = -y_{ji}$ is the flow over link $l = i \sim j$ from node i to j. Thus, if node i is neither the source node a nor the sink node b, then the net flow, the sum of the flows, at node i is zero. Each link $l = i \sim j$ between node i and j contains a resistor r_{ij}. A flow y_{ij} is said to be physical if there is an associated potential function v on the nodes of the network such that

$$v_i - v_j = r_{ij}y_{ij} \tag{7.19}$$

In electrical networks, the potential function is called the "voltage", whereas in hydraulic networks, it is called the "pressure". The relation (7.19), known as the law of Ohm, reflects that the potential difference $v_i - v_j$ generates a force that drives the current y_{ij} from node i to node j (if $v_i - v_j > 0$, else in the opposite direction) and that the potential difference is proportional to the current y_{ij}. The proportionality constant equals r_{ij}, the resistance between node i and j. For other electrical network elements such as capacitors and inductances, the relations between potential and current are more complicated than Ohm's law (7.19) and can be derived from the laws of Maxwell.

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[5] Simulations show that the relation is weakly concave.

Confining ourselves to a connected resistor network in which the flows are entirely specified by the conservation law (7.18) and Ohm's law (7.19), we will now translate the flow problem into a graph theoretical setting. The aim is to determine the effective resistance matrix Ω with elements ω_{ab} that satisfy $v_a - v_b = \omega_{ab}I$. The effective graph resistance, defined as

$$R_G = \frac{1}{2}\sum_{a=1}^{N}\sum_{b=1}^{N}\omega_{ab} = \frac{1}{2}u^T\Omega u \qquad (7.20)$$

can be regarded as a graph metric that measures the difficulty of transport in a graph G. Since the flow injected in node a can spread out over multiple paths towards node b, Klein and Randić (1993) characterize the effective graph resistance R_G by the "multiple route distance diminishment" feature, which is sometimes desirable over the conventional distance that uses a single path from a to b. Intuitively, even with two paths of different length, the robustness of communication between a and b might be enhanced somewhat by the longer path. The effective resistance ω_{ab} is a generalization to any configuration of the classical series and parallel formulas for the resistance.

Substituting Ohm's law (7.19) into the conservation law (7.18) yields

$$I\left(1_{\{i=a\}} - 1_{\{i=b\}}\right) = \sum_{j=1}^{N}\frac{a_{ij}}{r_{ij}}\left(v_i - v_j\right)$$

$$= v_i\sum_{j=1}^{N}\frac{a_{ij}}{r_{ij}} - \sum_{j=1}^{N}\frac{a_{ij}}{r_{ij}}v_j$$

We introduce the weighted adjacency matrix W, defined in **art. 3**, with elements $w_{ij} = \frac{a_{ij}}{r_{ij}}$ and obtain

$$I\left(1_{\{i=a\}} - 1_{\{i=b\}}\right) = v_i\sum_{j=1}^{N}w_{ij} - \sum_{j=1}^{N}w_{ij}v_j$$

Since this relation holds for any node i, the linear set of all such equations is written in matrix form as

$$I(e_a - e_b) = \left\{\mathrm{diag}\left(\sum_{j=1}^{N}w_{ij}\right) - W\right\}v = \tilde{Q}v$$

where $\tilde{Q}$ is the weighted Laplacian (**art. 3**) and e_k is the basic vector with the m th component equal to $1_{\{m=k\}}$. Similar to the Laplacian Q, one may verify from the proof of Theorem 10 that the weighted Laplacian $\tilde{Q}$ has non negative eigenvalues and the smallest eigenvalue is zero, belonging to the eigenvector u (because $\tilde{Q}u = 0$ as follows from the definition). Clearly, for the standard choice of unit resistances, W and $\tilde{Q}$ reduce to the adjacency matrix A and the Laplacian Q of the graph G.

For the subsequent algebraic manipulations, there is no loss in generality when we limit ourselves to the Laplacian.

Due to the zero eigenvalue $\mu_N = 0$, the matrix equation $I(e_a - e_b) = Qv$ cannot be inverted. However, using the spectral decomposition $Q = X\text{diag}(\mu_k) X^T$ in **art.** 156, we have

$$\text{diag}(\mu_k) X^T v = IX^T (e_a - e_b)$$

which shows that the last equation corresponding to $\mu_N = 0$ can be omitted. This means that one of the potentials $v_1, v_2, \ldots, v_N$ can be chosen at will, which coincides physically with the fact that only the potential difference matters. The simplest way of omitting one equation and choosing one of the potentials as a reference, is to proceed with the symmetric $N \times N$ matrix $\widehat{Q} = \widehat{X}\text{diag}(\mu_k) \widehat{X}^T$ instead of Q, where the $N \times (N-1)$ matrix $\widehat{X}$ consists of all eigenvectors of Q, except for the eigenvector u belonging to eigenvalue $\mu_N = 0$ and the $(N-1) \times (N-1)$ diagonal matrix $\text{diag}(\mu_k)$ contains only the positive eigenvalues of Q. **Art.** 148 shows that $\widehat{Q}$ equals the adjoint matrix of Q with $\lambda = 0$. The orthogonality of the eigenvectors shows that $\widehat{X}^T \widehat{X} = I$ and the pseudo inversion now equals

$$v = \widehat{Q}^{-1} I (e_a - e_b) \tag{7.21}$$
$$= I\widehat{X}\text{diag}(\mu_k^{-1}) \widehat{X}^T (e_a - e_b)$$

We present another expression for the pseudo inverse $\widehat{Q}^{-1}$, the inverse of the Laplacian within the subspace orthogonal to the vector u. **Art.** 85 shows that $\widehat{Q}^{-1} Q = Q\widehat{Q}^{-1} = Y$, where $Y = I - \frac{1}{N}J$ is the projection of any vector orthogonal to the vector u. Since $\widehat{Q}^{-1} J = \widehat{X}\text{diag}(\mu_k^{-1}) \widehat{X}^T u.u^T = 0$, we have that

$$\widehat{Q}^{-1}(Q + J) = Y = I - \frac{1}{N}J$$

and the matrix $Q + J$ has an inverse for any connected graph (**art.** 86). Thus,

$$\widehat{Q}^{-1} = (Q + J)^{-1} - \frac{1}{N}J(Q + J)^{-1}$$

Art. 84 shows that $J(Q + J)^{-1} = \frac{1}{N}J$ so that the pseudo inverse equals

$$\widehat{Q}^{-1} = (Q + J)^{-1} - \frac{1}{N^2}J$$

The definition $v_a - v_b = \omega_{ab}I$ and $v_a - v_b = (e_a - e_b)^T v$ combined with (7.21) then leads to the quadratic form

$$\omega_{ab} = (e_a - e_b)^T \widehat{Q}^{-1} (e_a - e_b)$$

Multiplying out yields

$$\omega_{ab} = \left(\widehat{Q}^{-1}\right)_{aa} + \left(\widehat{Q}^{-1}\right)_{bb} - 2\left(\widehat{Q}^{-1}\right)_{ab}$$

from which the symmetric effective resistance matrix Ω is obtained as

$$\Omega = z.u^T + u.z^T - 2\widehat{Q}^{-1} \tag{7.22}$$

where the vector $z = \left(\left(\widehat{Q}^{-1}\right)_{11}, \left(\widehat{Q}^{-1}\right)_{22}, \ldots, \left(\widehat{Q}^{-1}\right)_{NN}\right)$ and all diagonal elements of Ω are zero, as follows from the definition $v_a - v_b = \omega_{ab}I$. Finally, the effective graph resistance (7.20) equals

$$R_G = \frac{1}{2}u^T\Omega u = \frac{1}{2}u^T z.u^T u + \frac{1}{2}u^T u.z^T u - u^T\widehat{Q}^{-1}u$$
$$= Nu^T z = N\text{trace}\left(\widehat{Q}^{-1}\right)$$

because $u^T\widehat{Q}^{-1}u = u^T\widehat{X}\text{diag}(\mu_k^{-1})\,\widehat{X}^T u = 0$ as the vector u is orthogonal to each other eigenvector x_k of Q. Using (8.7) leads to the spectral expression for the effective graph resistance

$$R_G = N\sum_{k=1}^{N-1}\frac{1}{\mu_k} \tag{7.23}$$

For example, for the undirected version of the graph in Fig. 2.1, the effective resistance matrix Ω, computed from (7.22), is

$$\Omega = \begin{bmatrix} 0 & \frac{31}{66} & \frac{37}{66} & \frac{32}{33} & \frac{49}{66} & \frac{6}{11} \\ \frac{31}{66} & 0 & \frac{17}{33} & \frac{5}{6} & \frac{17}{33} & \frac{31}{66} \\ \frac{37}{66} & \frac{17}{33} & 0 & \frac{15}{22} & \frac{8}{11} & \frac{49}{66} \\ \frac{32}{33} & \frac{5}{6} & \frac{15}{22} & 0 & \frac{15}{22} & \frac{32}{33} \\ \frac{49}{66} & \frac{17}{33} & \frac{8}{11} & \frac{15}{22} & 0 & \frac{37}{66} \\ \frac{6}{11} & \frac{31}{66} & \frac{49}{66} & \frac{32}{33} & \frac{37}{66} & 0 \end{bmatrix}$$

and the corresponding effective graph resistance (7.23) is $R_G = \frac{659}{66} \simeq 9.98485$. A much more interesting example is the effective resistance of the chain of cliques $G_D^*(n_1, n_2, ..., n_{D+1})$, defined in Section 5.11. By using Theorem 27, **art.** 87 and the explicit relations for the coefficients $c_2(D)$ and $c_1(D)$ of the characteristic polynomial $p_D(\mu)$ in Van Mieghem and Wang (2009), the effective resistance of the chain of cliques $G_D^*(n_1, n_2, ..., n_{D+1})$ is

$$R_{G_D^*} = \sum_{q=2}^{D+1}\frac{\left(N - \sum_{k=1}^{q-1}n_k\right)}{n_{q-1}n_q}\sum_{k=1}^{q-1}n_k + N\sum_{k=1}^{D+1}\frac{n_k - 1}{n_{k-1} + n_k + n_{k+1}} \tag{7.24}$$

where the number of nodes N and the number of links L is given in (5.20) and (5.21) respectively. Theorem 23 shows that the minimum effective resistance in any graph with N nodes and diameter D is achieved in the class $G_D^*(n_1, n_2, ..., n_{D+1})$. Hence, minimizing (7.24) with respect to $n_1, n_2, \ldots, n_{D+1}$ subject to (5.20) yields the smallest possible effective resistance in any graph with N nodes and diameter D. An extreme case is the D hop line topology (see the end of Section 5.11), for

which all $n_j = 1$ such that $N = D + 1$ and the effective graph resistance, computed via (7.24) and via (7.23) with (5.9), is

$$R_{D\text{-hop line}} = \frac{D(D+1)(D+2)}{6} = \frac{D+1}{2} \sum_{k=1}^{D} \frac{1}{1 - \cos \frac{k\pi}{D+1}}$$

We end this section by establishing a lower and upper bound for the effective graph resistance R_G. **Art.** 87 demonstrates that

$$R_G = \frac{c_2(Q)}{\xi(G)} \geq \frac{(N-1)^2}{E[D]} \tag{7.25}$$

where the complexity $\xi(G)$ of the graph G equals the number of all possible spanning trees in the graph and where $c_2(Q)$ equals the number of all spanning trees with $N - 2$ links in all subgraphs of G that are obtained after deleting any pair of two nodes in G. The lower bound in (7.25) for the effective graph resistance R_G is attained by the complete graph K_N, for which $R_G = N - 1$. An upper bound follows from the physical fact that the effective resistance ω_{ab} is never larger than the sum of the resistances in the shortest path from a to b such that $\omega_{ab} \leq H_{ab}$, where the distance matrix H is defined in **art.** 3. This bound $\omega_{ab} \leq H_{ab}$ in (7.20) yields

$$R_G \leq \binom{N}{2} E[H]$$

where $E[H]$ is the average hopcount in the graph. Alternatively, this bound is equivalent to

$$E[H] \geq \frac{2}{N-1} \sum_{k=1}^{N-1} \frac{1}{\mu_k} \tag{7.26}$$

where equality is obtained for a tree as shown in (4.16) of **art.** 87.

Part II
Eigensystem and polynomials

8

Eigensystem of a matrix

This chapter reviews general results from linear algebra. In depth analyses are found in classical books by Gantmacher (1959a,b), Wilkinson (1965) and Meyer (2000). We refer to Golub and Van Loan (1996) for matrix computational methods and algorithms.

In this chapter, A is a general matrix, not the adjacency matrix.

8.1 Eigenvalues and eigenvectors

138. The algebraic eigenproblem consists in the determination of the eigenvalues λ and the corresponding eigenvectors x of an $n \times n$ matrix A for which the set of n homogeneous linear equations in n unknowns,

$$Ax = \lambda x \tag{8.1}$$

has a non zero solution. Clearly, the zero vector $x = 0$ is always a solution of (8.1). A non zero solution of (8.1) is only possible if and only if the matrix $A - \lambda I$ is singular, that is,

$$\det (A - \lambda I) = 0 \tag{8.2}$$

This determinant can be expanded in a polynomial in λ of degree n,

$$c_A(\lambda) = \sum_{k=0}^{n} c_k \lambda^k = c_n \lambda^n + c_{n-1} \lambda^{n-1} + \cdots + c_1 \lambda + c_0 = 0 \tag{8.3}$$

which is called the characteristic or eigenvalue polynomial of the matrix A. Apart from $c_n = (-1)^n$, the coefficients for $0 \leq k < n$ are

$$c_k = (-1)^k \sum_{all} M_{n-k} \tag{8.4}$$

and M_k is a principal minor[1]. Since a polynomial of degree n has n complex zeros

---

[1] A principal minor M_k is the determinant of a principal $k \times k$ submatrix $M_{k \times k}$ obtained by deleting the same $n-k$ rows and columns in A. Hence, the main diagonal elements $(M_{k \times k})_{ii}$ are k elements of main diagonal elements $\{a_{ii}\}_{1 \leq i \leq n}$ of A.

(**art.** 196), the matrix A possesses n eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_1$, not all necessarily distinct. In general, the characteristic polynomials can be written as

$$c_A(\lambda) = \prod_{k=1}^{n} (\lambda_k - \lambda) \qquad (8.5)$$

Since $c_A(\lambda) = \det(A - \lambda I)$, it follows from (8.3) and (8.5) that, for $\lambda = 0$,

$$\det A = c_0 = \prod_{k=1}^{n} \lambda_k \qquad (8.6)$$

Hence, if $\det A = 0$, there is at least one zero eigenvalue. Also,

$$(-1)^{n-1} c_{n-1} = \sum_{k=1}^{n} \lambda_k = \text{trace}(A) \qquad (8.7)$$

and

$$c_1 = -\sum_{k=1}^{n} \prod_{j=1;j\neq k}^{n} \lambda_j = -\det A \sum_{k=1}^{n} \frac{1}{\lambda_k} \qquad (8.8)$$

For any eigenvalue λ, the set (8.1) has at least one non zero eigenvector x. Fur thermore, if x is a non zero eigenvector, also kx is a non zero eigenvalue. Therefore, eigenvectors are often normalized, for instance, a probabilistic eigenvector has the sum of its components equal to 1 or a norm $\|x\|_1 = 1$ as defined in (8.39).

If the rank of $A - \lambda I$ is less than $n - 1$, there will be more than one independent vector. Just these cases seriously complicate the eigenvalue problem. In the sequel, we omit the discussion on multiple eigenvalues and refer to Wilkinson (1965).

139. *General bounds on the position of eigenvalues.*

Theorem 36 (Gerschgorin) *Every eigenvalue of a matrix A lies in at least one of the circular discs with center a_{jj} and radii $R_j = \sum_{k=1;k\neq j} |a_{jk}|$ or $r_j = \sum_{k=1;k\neq j} |a_{kj}|$*

Proof: Suppose that the r th component of the eigenvector x of A belonging to eigenvalue λ has the largest modulus. An eigenvector can always be scaled and we normalize such that

$$x^T = (x_1, x_2, \ldots, x_{r-1}, 1, x_{r+1}, \ldots, x_n)$$

where $|x_j| \leq 1$, for all j. Equating the r th component on both sides of the eigenvalue equation $Ax = \lambda x$ gives

$$\sum_{k=1}^{n} a_{rk} x_k = \lambda x_r = \lambda$$

Hence,

$$|a_{rr} - \lambda| \le \sum_{k=1;k\ne r}^{n} |a_{rk} x_k| \le \sum_{k=1;k\ne r}^{n} |a_{rk}|\,|x_k| \le \sum_{k=1;k\ne r}^{n} |a_{rk}|$$

which shows that λ lies in a circular disc centered at a_{rr} with a radius not larger than $\sum_{k=1;k\ne r}^{n} |a_{rk}|$. The other radius mentioned follows from the fact that A and A^T have the same eigenvalues as shown in **art.** 140. $\qquad\square$

140. The eigenproblem of the transpose A^T,

$$A^T y = \lambda y \tag{8.9}$$

is of singular importance. Since the determinant of a matrix is equal to the de terminant of its transpose, $\det\left(A^T - \lambda I\right) = \det\left(A - \lambda I\right)$, which shows that the eigenvalues of A and A^T are the same. However, the eigenvectors are, in general, different. Alternatively, transposing (8.9) yields

$$y^T A = \lambda y^T \tag{8.10}$$

The vector y_j^T is therefore called the left eigenvector of A belonging to the eigenvalue λ_j, whereas x_j is called the right eigenvector belonging to the same eigenvalue λ_j. An important relation between the left and right eigenvectors of a matrix A is, for $\lambda_j \ne \lambda_k$,

$$y_j^T x_k = 0 \tag{8.11}$$

Indeed, left multiplying (8.1) with $\lambda = \lambda_k$ by y_j^T,

$$y_j^T A x_k = \lambda_k y_j^T x_k$$

and similarly right multiplying (8.10) with $\lambda = \lambda_j$ by x_k

$$y_j^T A x_k = \lambda_j y_j^T x_k$$

leads, after subtraction to $0 = (\lambda_k - \lambda_j)\, y_j^T x_k$ and (8.11) follows. Since eigenvectors may be complex in general and since $y_j^T x_k = x_k^T y_j$, the expression $y_j^T x_k$ is not an inner product that is always real and for which $y_j^T x_k = \left(x_k^T y_j\right)^*$ holds. However, (8.11) expresses that the sets of left and right eigenvectors are orthogonal if $\lambda_j \ne \lambda_k$.

141. If A has n distinct eigenvalues, then the n eigenvectors are linearly inde pendent and span the whole n dimensional space. The proof is by *reductio ad absurdum*. Assume that s is the smallest number of linearly dependent eigenvectors labelled by the first s smallest indices. Linear dependence then means that

$$\sum_{k=1}^{s} \alpha_k x_k = 0 \tag{8.12}$$

where $\alpha_k \neq 0$ for $1 \leq k \leq s$. Left multiplying by A and using (8.1) yields

$$\sum_{k=1}^{s} \alpha_k \lambda_k x_k = 0 \tag{8.13}$$

On the other hand, multiplying (8.12) by λ_s and subtracting from (8.13) leads to

$$\sum_{k=1}^{s-1} \alpha_k \left(\lambda_k - \lambda_s\right) x_k = 0,$$

which, because all eigenvalues are distinct, implies that there is a smaller set of $s-1$ linearly depending eigenvectors. This contradicts the initial hypothesis.

This important property has a number of consequences. First, it applies to left as well as to right eigenvectors. Relation (8.11) then shows that the sets of left and right eigenvectors form a bi orthogonal system with $y_k^T x_k \neq 0$. For, if x_k were orthogonal to y_k (or $y_k^T x_k = 0$), (8.11) demonstrates that x_k would be orthogonal to all left eigenvectors y_j. Since the set of left eigenvectors span the n dimensional vector space, it would mean that the n dimensional vector x_k would be orthogonal to the whole n space, which is impossible because x_k is not the null vector. Second, any n dimensional vector can be written in terms of either the left or right eigenvectors.

142. Let us denote by X the matrix with the right eigenvector x_j in column j and by Y^T the matrix with the left eigenvector y_k^T in row k. If the right and left eigenvectors are scaled such that, for all $1 \leq k \leq n$, $y_k^T x_k = 1$, then

$$Y^T X = I \tag{8.14}$$

or the matrix Y^T is the inverse of the matrix X. Furthermore, for any right eigenvector, (8.1) holds, rewritten in matrix form, such that

$$AX = X \, \text{diag}(\lambda_k) \tag{8.15}$$

Left multiplying by $X^{-1} = Y^T$ yields the similarity transform of matrix A,

$$X^{-1}AX = Y^T AX = \text{diag}(\lambda_k) \tag{8.16}$$

Thus, when the eigenvalues of A are distinct, there exists a similarity transform $H^{-1}AH$ that reduces A to diagonal form. In many applications, similarity transforms are applied to simplify matrix problems. Observe that a similarity transform preserves the eigenvalues, because, if $Ax = \lambda x$, then $\lambda H^{-1}x = H^{-1}Ax = (H^{-1}AH)H^{-1}x$. The eigenvectors are transformed to $H^{-1}x$.

When A has multiple eigenvalues, it may be impossible to reduce A to a diagonal form by similarity transforms. Instead of a diagonal form, the most compact form when A has r distinct eigenvalues each with multiplicity m_j such that $\sum_{j=1}^{r} m_j = n$

is the Jordan canonical form C,

$$
C =
\begin{bmatrix}
C_{m_1\ a}(\lambda_1) & & & & \\
& C_a(\lambda_1) & & & \\
& & \vdots & & \\
& & & C_{m_{r\ 1}}(\lambda_{r\ 1}) & \\
& & & & C_{m_r}(\lambda_r)
\end{bmatrix}
$$

where $C_m(\lambda)$ is an $m \times m$ submatrix of the form

$$
C_m(\lambda) =
\begin{bmatrix}
\lambda & 1 & 0 & \cdots & 0 \\
0 & \lambda & 1 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & \lambda & 1 \\
0 & \cdots & 0 & 0 & \lambda
\end{bmatrix}
$$

The number of independent eigenvectors is equal to the number of submatrices. If an eigenvalue λ has multiplicity m, there can be one large submatrix $C_m(\lambda)$, but also a number k of smaller submatrices $C_{b_j}(\lambda)$ such that $\sum_{j=1}^{k} b_j = m$. This illustrates, as mentioned in **art.** 138, the much higher complexity of the eigenproblem in case of multiple eigenvalues. For more details we refer to Wilkinson (1965).

143. The companion matrix of a polynomial $p_n(\lambda) = \sum_{k=0}^{n} a_k z^k$ is defined as

$$
C =
\begin{bmatrix}
-\frac{a_{n\ 1}}{a_n} & -\frac{a_{n\ 2}}{a_n} & \cdots & -\frac{a_1}{a_n} & -\frac{a_0}{a_n} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{bmatrix}
$$

although other variants also appear in the literature, such as

$$
C =
\begin{bmatrix}
0 & 0 & \cdots & 0 & -\frac{a_0}{a_n} \\
1 & 0 & \cdots & 0 & -\frac{a_1}{a_n} \\
0 & 1 & \cdots & 0 & -\frac{a_2}{a_n} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & -\frac{a_{n\ 1}}{a_n}
\end{bmatrix}
$$

The basic property of the companion matrix C is

$$
\det(C - \lambda I) = (-1)^n \frac{p_n(\lambda)}{a_n} \tag{8.17}
$$

Indeed, in

$$\det(C - \lambda I) = \begin{vmatrix} -\frac{a_{n-1}}{a_n} - \lambda & -\frac{a_{n-2}}{a_n} & \cdots & -\frac{a_1}{a_n} & -\frac{a_0}{a_n} \\ 1 & -\lambda & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -\lambda \end{vmatrix}$$

multiply the first column by λ^{n-1}, the second column by λ^{n-2}, and so on, and add them to the last column. The resulting last column elements are zero, except for that in the first row, which is $-\frac{p_n(\lambda)}{a_n}$. The corresponding cofactor is one, which proves (8.17). From (9.2), **art.** 144 and (8.17), it follows that the inverse of the companion matrix C is

$$C^{-1} = \begin{bmatrix} -\frac{a_1}{a_0} & -\frac{a_2}{a_0} & \cdots & -\frac{a_{n-1}}{a_0} & -\frac{a_n}{a_0} \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

The companion matrix of the characteristic polynomial (8.3) of A is defined as

$$C = \begin{bmatrix} (-1)^{n-1}c_{n-1} & (-1)^{n-1}c_{n-2} & \cdots & (-1)^{n-1}c_1 & (-1)^{n-1}c_0 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

such that $\det(C - \lambda I) = c_A(\lambda)$. If A has distinct eigenvalues, A as well as C are similar to $\mathrm{diag}(\lambda_i)$. It has been shown in **art.** 142 that the similarity transform H for A equals $H = X$. The similarity transform for C is the Vandermonde matrix $V_n(\lambda)$, where

$$V_n(x) = \begin{bmatrix} x_1^{n-1} & x_2^{n-1} & \cdots & x_{n-1}^{n-1} & x_n^{n-1} \\ x_1^{n-2} & x_2^{n-2} & \cdots & x_{n-1}^{n-2} & x_n^{n-2} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ x_1 & x_2 & \vdots & x_{n-1} & x_n \\ 1 & 1 & \cdots & 1 & 1 \end{bmatrix}$$

Furthermore,

$$
V_n(\lambda)\mathrm{diag}(\lambda_i) =
\begin{bmatrix}
\lambda_1^{n} & \lambda_2^{n} & \cdots & \lambda_{n-1}^{n} & \lambda_n^{n} \\
\lambda_1^{n-1} & \lambda_2^{n-1} & \cdots & \lambda_{n-1}^{n-1} & \lambda_n^{n-1} \\
\vdots & \vdots & \cdots & \vdots & \vdots \\
\lambda_1^{2} & \lambda_2^{2} & \vdots & \lambda_{n-1}^{2} & \lambda_n^{2} \\
\lambda_1 & \lambda_2 & \cdots & \lambda_{n-1} & \lambda_n
\end{bmatrix}
$$

while

$$
CV_n(\lambda) =
\begin{bmatrix}
(-1)^{n-1}c_A(\lambda_1)+\lambda_1^{n} & (-1)^{n-1}c_A(\lambda_2)+\lambda_2^{n} & \cdots & (-1)^{n-1}c_A(\lambda_n)+\lambda_n^{n} \\
\lambda_1^{n-1} & \lambda_2^{n-1} & \cdots & \lambda_n^{n-1} \\
\vdots & \vdots & \cdots & \vdots \\
\lambda_1^{2} & \lambda_2^{2} & \vdots & \lambda_n^{2} \\
\lambda_1 & \lambda_2 & \cdots & \lambda_n
\end{bmatrix}
$$

Since $c_A(\lambda_j) = 0$, it follows that $CV_n(\lambda) = V_n(\lambda)\mathrm{diag}(\lambda_i)$, which demonstrates the claim. Hence, the eigenvector x_k of C belonging to eigenvalue λ_k is

$$
x_k^T = \begin{bmatrix} \lambda_k^{n-1} & \lambda_k^{n-2} & \cdots & \lambda_k & 1 \end{bmatrix}
$$

The Vandermonde matrix $V_n(\lambda)$ is clearly non singular if all eigenvalues are distinct (see also **art. 194**). In the case that $\det V_n(\lambda) \neq 0$, the matrix $V_n(\lambda)$ is of rank n, implying that all eigenvectors are linearly independent. The eigenvectors are only orthogonal if $x_k^T x_m = 0$ for each pair (k, m) with $k \neq m$. In other words, if

$$
0 = \sum_{j=1}^{n} (\lambda_k)^j (\lambda_m)^j = \lambda_k \lambda_m \frac{(\lambda_k \lambda_m)^n - 1}{\lambda_k \lambda_m - 1}
$$

The solution is $\lambda_k \lambda_m = e^{\frac{2\pi i l}{n}}$ for $l = 1, 2, \ldots, n-1$, which implies that each of the n eigenvalues $\{\lambda_k\}_{1 \leq k \leq n}$ must be a n th distinct root of unity and that the associated polynomial to the companion matrix is $p_n(z) = a_n(z^n \pm 1)$.

The first component or row in the eigenvalue equation $Cx = \lambda x$ expresses explicitly the root equation $c_A(\lambda) = 0$ of the polynomial

$$
(Cx_k)_1 - (\lambda_k x_k)_1 = -c_A(\lambda_k) = 0 \tag{8.18}
$$

and any other row is an identity. If C has an eigenvalue λ_k of multiplicity m, then λ_k satisfies $c_A(\lambda_k) = c_A'(\lambda_k) = \ldots = c_A^{(m-1)}(\lambda_k) = 0$. The first equality is equivalent to (8.18). The others are similarly derived by differentiating (8.18) with respect to λ_k such that, for $1 \leq j \leq m-1$,

$$
\left(Cx_k^{(j)}\right)_1 - \left(jx_k^{(j-1)}\right)_1 - \left(\lambda_k x_k^{(j)}\right)_1 = -c_A^{(j)}(\lambda_k) = 0
$$

Hence, if λ_k is a zero with multiplicity m, then $Cx_k = \lambda_k x_k$, where x_k is the eigenvector and the other $2 \leq j \leq m$ equations are

$$
Cy_j = \lambda_k y_j + y_{j-1}
$$

where $y_j = \frac{x_k^{(j-1)}}{(j-1)!}$ is a generalized eigenvector,

$$y_j^T = \begin{bmatrix} 0 & 0 & \cdots & 1 & \binom{j}{j-1}\lambda_k & \cdots & \binom{n-1}{j-1}\lambda_k^{n-j} \end{bmatrix}$$

which has a 1 in the j th position. Clearly, with this notation, $x_k = y_1$. More over, the set of the eigenvector and $m-1$ generalized eigenvectors are independent because the $m \times n$ matrix formed by their components has rank m.

144. When left multiplying (8.1), we obtain

$$A^2 x = \lambda A x = \lambda^2 x$$

and, in general for any integer $k \geq 0$,

$$A^k x = \lambda^k x \tag{8.19}$$

Moreover, if A has no zero eigenvalue, i.e., A^{-1} exists, then left multiplying (8.1) with A^{-1} yields

$$A^{-1} x = \lambda^{-1} x$$

We apply (8.19) to the matrix A^{-1} and conclude that

$$A^{-k} x = \lambda^{-k} x$$

In other words, if the inverse matrix A^{-1} exists, then equation (8.19) is valid for any integer, positive as well as negative.

Combining (8.19) and (8.7) implies that

$$\text{trace}\left(A^k\right) = \sum_{j=1}^{n} \lambda_j^k (A) \tag{8.20}$$

145. *The Caley Hamilton Theorem.* Since any eigenvalue λ satisfies its character istic polynomial $c_A (\lambda) = 0$, we directly find from (8.19) that the matrix A satisfies its own characteristic equation,

$$c_A(A) = O \tag{8.21}$$

This result is the Caley Hamilton Theorem. There exist several other proofs of the Caley Hamilton Theorem.

Let $m_{c_A} (z) = \sum_{k=0}^{l} b_k z^k$ denote the minimal polynomial, defined in **art. 211**, of the characteristic polynomial $c_A (z)$ of a matrix A and the degree of the minimal polynomial obeys $l \leq n$, where l are the number of different eigenvalues of A. Any eigenvalue λ of the matrix A satisfies $m_{c_A} (\lambda) = 0$. Analogously as for the Caley Hamilton Theorem, we also have from (8.19) that

$$m_{c_A} (A) = O$$

Clearly, if $F (z)$ is any polynomial satisfying $F (A) = O$, then $m_{c_A} (z) | F (z)$ as well as $m_{c_A} (z) | c (z)$.

146. *Power method.* Let $x_1, x_2, \ldots, x_n$ denote the eigenvectors of A belonging to the distinct eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. **Art.** 141 demonstrates that this set of linearly independent vectors spans the n dimensional space such that any other vector w can be written as a linear combination,

$$w = \sum_{j=1}^{n} \alpha_j x_j$$

Then, for any integer k and using (8.19) yields

$$A^k w = \sum_{j=1}^{n} \alpha_j A^k x_j = \sum_{j=1}^{n} \alpha_j \lambda_j^k x_j$$

If the largest eigenvalue obeys that $|\lambda_1| > |\lambda_2|$ and $|\lambda_2| \geq |\lambda_j|$ for any $3 \leq j \leq n$, then, for large k, we observe that

$$A^k w = \alpha_1 \lambda_1^k x_1 \left(1 + O\left(\left(\frac{|\lambda_2|}{|\lambda_1|} \right)^k \right) \right)$$

This shows that, after subsequent multiplications with A, an arbitrary vector w aligns increasingly more towards the largest eigenvector x_1. This so called power method lies at the basis of the computations of the largest eigenvector, especially in large and sparse matrices. In particular, the sequence $Aw, A^2 w, A^4 w, \ldots, A^{2^m} w$, tends exponentially fast to a vector, proportional to the largest eigenvector x_1 of A (under the very mild condition that $|\lambda_1| > |\lambda_2|$).

8.2 Functions of a matrix

147. Consider an arbitrary matrix polynomial in λ,

$$F(\lambda) = \sum_{k=0}^{m} F_k \lambda^k$$

where all F_k are $n \times n$ matrices and $F_m \neq O$. Any matrix polynomial $F(\lambda)$ can be right and left divided by another (non zero) matrix polynomial $B(\lambda)$ in a unique way as proved in Gantmacher (1959a, Chapter IV). Hence the left quotient and left remainder $F(\lambda) = B(\lambda)Q_L(\lambda) + L(\lambda)$ and the right quotient and right remainder $F(\lambda) = Q_R(\lambda)B(\lambda) + R(\lambda)$ are unique. Let us concentrate on the right remainder in the case where $B(\lambda) = \lambda I - A$ is a linear polynomial in λ. Using Euclid's division

scheme for polynomials (**art.** 208),

$$F(\lambda) = F_m\lambda^{m-1}(\lambda I - A) + (F_m A + F_{m-1})\lambda^{m-1} + \sum_{k=0}^{m-2} F_k\lambda^k$$

$$= \left[F_m\lambda^{m-1} + (F_m A + F_{m-1})\lambda^{m-2}\right](\lambda I - A)$$

$$+ \left(F_m A^2 + F_{m-1}A + F_{m-2}\right)\lambda^{m-2} + \sum_{k=0}^{m-3} F_k\lambda^k$$

and continuing, we arrive at

$$F(\lambda) = \left[F_m\lambda^{m-1} + \cdots + \lambda^{k-1}\sum_{j=k}^{m} F_j A^{j-k} + \cdots + \sum_{j=1}^{m} F_j A^{j-1}\right](\lambda I - A)$$

$$+ \sum_{j=0}^{m} F_j A^j$$

In summary, $F(\lambda) = Q_R(\lambda)(\lambda I - A) + R(\lambda)$ (and similarly for the left quotient and left remainder) with

$$\begin{array}{ll}
Q_R(\lambda) = \sum_{k=1}^{m}\lambda^{k-1}\left(\sum_{j=k}^{m} F_j A^{j-k}\right) & Q_L(\lambda) = \sum_{k=1}^{m}\lambda^{k-1}\left(\sum_{j=k}^{m} A^{j-k}F_j\right) \\
R(\lambda) = \sum_{j=0}^{m} F_j A^j = F(A) & L(\lambda) = \sum_{j=0}^{m} A^j F_j
\end{array}$$

$$(8.22)$$

and where the right remainder is independent of λ. The Generalized Bézout Theorem states that the polynomial $F(\lambda)$ is divisible by $(\lambda I - A)$ on the right (left) if and only if $F(A) = O$ $(L(\lambda) = O)$.

148. *The adjoint matrix.* By the Generalized Bézout Theorem, the polynomial $F(\lambda) = g(\lambda)I - g(A)$ is divisible by $(\lambda I - A)$ because $F(A) = g(A)I - g(A) = O$. If $F(\lambda)$ is an ordinary polynomial, the right and left quotient and remainder are equal. The Caley Hamilton Theorem (8.21) states that $c_A(A) = 0$, which indicates that $c_A(\lambda)I = Q(\lambda)(\lambda I - A)$ and also $c_A(\lambda)I = (\lambda I - A)Q(\lambda)$. The matrix

$$Q(\lambda) = (\lambda I - A)^{-1} c_A(\lambda)$$

is called the adjoint matrix of A. Explicitly, from (8.22),

$$Q(\lambda) = \sum_{k=1}^{n}\lambda^{k-1}\left(\sum_{j=k}^{n} c_j A^{j-k}\right)$$

and, with (8.6),

$$Q(0) = -(A)^{-1}\det A = \sum_{j=1}^{n} c_j A^{j-1}$$

The main theoretical interest of the adjoint matrix stems from its definition,

$$c_A(\lambda)I = Q(\lambda)(\lambda I - A) = (\lambda I - A)Q(\lambda)$$

In case $\lambda = \lambda_k$ is an eigenvalue of A, then $(\lambda_k I - A) Q(\lambda_k) = 0$, which indicates by (8.1) and the commutative property $(\lambda I - A) Q(\lambda) = Q(\lambda) (\lambda I - A)$ that every non zero column(row) of the adjoint matrix $Q(\lambda_k)$ is a right(left) eigenvector belonging to the eigenvalue λ_k. In addition, by differentiation with respect to λ, we obtain

$$c'_A(\lambda)I = (\lambda I - A) Q'(\lambda) + Q(\lambda)$$

This demonstrates that, if $Q(\lambda_k) \neq O$, the eigenvalue λ_k is a simple root of $c_A(\lambda)$ and, conversely, if $Q(\lambda_k) = O$, the eigenvalue λ_k has higher multiplicity.

The adjoint matrix $Q(\lambda) = (\lambda I - A)^{-1} c_A(\lambda)$ is computed by observing that, on the Generalized Bézout Theorem, $\frac{c_A(\lambda)}{\lambda} \frac{c_A(\mu)}{\mu}$ is divisible without remainder. By replacing λ and μ in this polynomial by λI and A respectively, $Q(\lambda)$ readily follows.

149. Consider the arbitrary polynomial of degree l,

$$g(x) = g_0 \prod_{j=1}^{l} (x - \mu_j)$$

Substitute x by A, then

$$g(A) = g_0 \prod_{j=1}^{l} (A - \mu_j I)$$

Since $\det(AB) = \det A \det B$ and $\det(kA) = k^n \det A$, we have

$$\det(g(A)) = g_0^n \prod_{j=1}^{l} \det(A - \mu_j I) = g_0^n \prod_{j=1}^{l} c(\mu_j)$$

With (8.5),

$$\det(g(A)) = g_0^n \prod_{j=1}^{l} \prod_{k=1}^{n} (\lambda_k - \mu_j) = \prod_{k=1}^{n} g_0 \prod_{j=1}^{l} (\lambda_k - \mu_j)$$

$$= \prod_{k=1}^{n} g(\lambda_k)$$

If $h(x) = g(x) - \lambda$, we arrive at the general result: for any polynomial $g(x)$, the eigenvalues of $g(A)$ are $g(\lambda_1), \ldots, g(\lambda_n)$ and the characteristic polynomial is

$$\det(g(A) - \lambda I) = \prod_{k=1}^{n} (g(\lambda_k) - \lambda) \tag{8.23}$$

which is a polynomial in λ of degree at most n. Since the result holds for an arbitrary polynomial, it should not surprise that, under appropriate conditions of convergence, it can be extended to infinite polynomials, in particular to the Taylor series of a complex function. As proved in Gantmacher (1959a, Chapter V), if the

power series of a function $f(z)$ around $z = z_0$,

$$f(z) = \sum_{j=1}^{\infty} f_j(z_0)(z - z_0)^j \qquad (8.24)$$

converges for all z in the disc $|z - z_0| < R$, then $f(A) = \sum_{j=1}^{\infty} f_j(z_0)(A - z_0 I)^j$ provided that all eigenvalues of A lie within the region of convergence of (8.24), i.e., $|\lambda - z_0| < R$. For example,

$$e^{Az} = \sum_{k=0}^{\infty} \frac{z^k A^k}{k!} \qquad \text{for all } A$$

$$\log A = \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \frac{1}{}(A - I)^k \text{ for } |\lambda_k - 1| < 1, \text{ all } 1 \le k \le n$$

and, from (8.23), the eigenvalues of e^{Az} are $e^{z\lambda_1}, \ldots, e^{z\lambda_1}$. Hence, the knowledge of the eigenstructure of a matrix A allows us to compute any function of A (under the same convergence restrictions as complex numbers z).

8.3 Hermitian and real symmetric matrices

150. *A Hermitian matrix.* A Hermitian matrix A is a complex matrix that obeys $A^H = (A^T)^* = A$, where $a^H = (a_{ij})^*$ is the complex conjugate of a_{ij}. The super script H, in honor of Charles Hermite, means to take the complex conjugate and then a transpose. Hermitian matrices possess a number of attractive properties. A particularly interesting subclass of Hermitian matrices are real, symmetric matrices that obey $A^T = A$. The inner product of vector y and x is defined as $y^H x$ and obeys $(y^H x)^* = (y^H x)^H = x^H y$. The inner product $x^H x = \sum_{j=1}^{n} |x_j|^2$ is real and positive for all vectors except for the null vector.

151. The eigenvalues of a Hermitian matrix are all real. Indeed, left multiplying (8.1) by x^H yields

$$x^H A x = \lambda x^H x$$

and, since $(x^H A x)^H = x^H A^H x = x^H A x$, it follows that $\lambda x^H x = \lambda^H x^H x$ or $\lambda = \lambda^H$ because $x^H x$ is a positive real number. Furthermore, since $A = A^H$, we have

$$A^H x = \lambda x$$

Taking the complex conjugate, yields

$$A^T x^* = \lambda x^*$$

In general, the eigenvectors of a Hermitian matrix are complex, but real for a real symmetric matrix since $A^H = A^T$. Moreover, the left eigenvector y^T is the

complex conjugate of the right eigenvector x. Hence, the orthogonality relation (8.11) reduces, after normalization, to the inner product

$$x_k^H x_j = \delta_{kj} \tag{8.25}$$

where δ_{kj} is the Kronecker delta, which is zero if $k \neq j$ and else $\delta_{kk} = 1$. Consequently, (8.14) reduces to

$$X^H X = I \tag{8.26}$$

which implies that the matrix X formed by the eigenvectors is an unitary matrix $(X^{-1} = X^H)$.

For a real symmetric matrix A, the corresponding relation $X^T X = I$ implies that X is an orthogonal matrix $(X^{-1} = X^T)$ obeying

$$X^T X = X X^T = I$$

where the first equality follows from the commutativity of the inverse of a matrix, $X^{-1} X = X X^{-1}$. Hence, all eigenvectors of a symmetric matrix are orthogonal. Although the arguments so far (see Section 8.1) have assumed that the eigenvalues of A are distinct, the theorem applies in general as proved in Wilkinson (1965, Section 47): for any Hermitian matrix A, there exists a unitary matrix U such that, for real λ_j,

$$U^H A U = \operatorname{diag}(\lambda_j)$$

and for any real symmetric matrix A, there exists an orthogonal matrix U such that, for real λ_j,

$$U^T A U = \operatorname{diag}(\lambda_j)$$

152. *The Rayleigh inequalities.* The normalized eigenvectors x_k and x_m of real symmetric[2] A obey $x_k^T A x_m = 0$ if $k \neq m$ and $x_k^T A x_k = \lambda_k$ (**art. 151**). These n eigenvectors span the n dimensional space. Let w be an $n \times 1$ vector that can be written as a linear combination of the first j eigenvectors of A,

$$w = c_1 x_1 + c_2 x_2 + \cdots + c_j x_j$$

where all $c_k \in \mathbb{R}$. Equivalently, $w \in \mathcal{X}_j$, where $\mathcal{X}_j$ is the space spanned by the vectors $\{x_1, x_2, \ldots, x_j\}$. Then $w^T w = \sum_{k=1}^{j} \sum_{m=1}^{j} c_k c_m x_k^T x_m = \sum_{k=1}^{j} c_k^2$ and

$$w^T A w = \sum_{k=1}^{j} \sum_{m=1}^{j} c_k c_m x_k^T A x_m = \sum_{k=1}^{j} c_k^2 \lambda_k$$

Since A has real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$, this ordering of the eigenvalues leads to the bound $\lambda_j \sum_{k=1}^{j} c_k^2 \leq \sum_{k=1}^{j} c_k^2 \lambda_k \leq \lambda_1 \sum_{k=1}^{j} c_k^2$ from which the Rayleigh inequalities for $w \in \mathcal{X}_j$ follow as

$$\lambda_j \leq \frac{w^T A w}{w^T w} \leq \lambda_1 \tag{8.27}$$

[2] The extension to a Hermitian matrix is straightforward and omitted.

Equality in $\frac{w^T A w}{w^T w} = \lambda_k$ is only attained provided $w \in \mathcal{X}_j$ is an eigenvector of A belonging to eigenvalue λ_k with $\lambda_j \le \lambda_k \le \lambda_1$. If w is a vector that is orthogonal to the first j eigenvectors of A, which means that $w = c_{j+1}x_{j+1} + c_{j+2}x_{j+2} + \cdots + c_n x_n$ can be written as a linear combination of the last $n-j$ eigenvectors or that $w \in \mathcal{X}_j^{\perp}$, then $\lambda_n \le \frac{w^T A w}{w^T w} \le \lambda_{j+1}$.

The two extreme eigenvalues can thus be written as

$$\lambda_1 = \sup_{y \ne 0} \frac{y^T A y}{y^T y} \tag{8.28}$$

$$\lambda_n = \inf_{y \ne 0} \frac{y^T A y}{y^T y} \tag{8.29}$$

153. *Complex symmetric matrix.* Let A be a complex symmetric matrix and x_k is the eigenvector belonging to eigenvalue λ_k,

$$A x_k = \lambda_k x_k$$

In general, both x_k and λ_k are complex. For example, the matrix $\mathrm{diag}(i\omega_k)$ with $\omega_k \in \mathbb{R}$ is symmetric and all its eigenvalues are purely imaginary. Since $A = A^T$ is symmetric, the right and left eigenvectors are the same and (8.14) shows that the matrix X with the eigenvectors placed in columns is orthogonal. This illustrates that the set of eigenvectors span the n dimensional space. Left multiplication with x_k^T gives

$$\lambda_k = \frac{x_k^T A x_k}{x_k^T x_k}$$

Also $x_k^T x_k$ is complex in general. Only when taking the absolute value, an ordering $|\lambda_1| \ge |\lambda_2| \ge \ldots \ge \lambda_n$ can be obtained and the same argument as in **art.** 152 leads to

$$|\lambda_n| \le \left| \frac{w^T A w}{w^T w} \right| \le |\lambda_1|$$

for any (complex) vector w.

Symmetry $A = A^T$ guarantees that the set of (possibly complex) eigenvectors is an orthogonal basis for the n dimensional space. If A is not symmetric, diagonalization via a similarity transform may not be possible (**art.** 142) so that Rayleigh's inequalities are not valid. For example, if A is an $n \times n$ upper triangular matrix with all ones and ones on the diagonal, then all eigenvalues are equal to 1, one eigenvector is $e_1 = (1, 0, \ldots, 0)$ and all others are zero. Choosing $w = u$ gives $\frac{u^T A u}{u^T u} = \frac{n+1}{2} > 1$ for $n > 1$, violating the Rayleigh inequality (8.27) for the largest eigenvalue.

154. *Field of values.* The field of values $\Phi(.)$ is a set of complex numbers associated to an $n \times n$ matrix A,

$$\Phi(A) = \left\{ x^H A x : x \in \mathbb{C}^n,\ x^H x = 1 \right\} \tag{8.30}$$

While the spectrum of a matrix is a discrete set, the field of values $\Phi\left(.\right)$, of which instances appeared in **art.** 152 and **art.** 153, can be a continuum. However, $\Phi\left(A\right)$ is always a convex subset of $\mathbb{C}$ for any matrix A, a fundamental fact known as the Toeplitz Hausdorff Theorem and proved in Horn and Johnson (1991, Section 1.3). Another property is the subadditivity, $\Phi\left(A+B\right)\subset\Phi\left(A\right)+\Phi\left(B\right)$, which follows from the definition (8.30). Indeed,

$$\begin{aligned}
\Phi\left(A+B\right) &= \left\{x^{H}Ax+x^{H}Bx:x\in\mathbb{C}^{n},\,x^{H}x=1\right\}\\
&\subset \left\{x^{H}Ax:x\in\mathbb{C}^{n},\,x^{H}x=1\right\}+\left\{y^{H}By:y\in\mathbb{C}^{n},\,y^{H}y=1\right\}\\
&= \Phi\left(A\right)+\Phi\left(B\right)
\end{aligned}$$

Since the set $\lambda\left(A\right)$ of eigenvalues of A belongs to $\Phi\left(A\right)$, it holds that

$$\lambda\left(A+B\right)\subset\Phi\left(A+B\right)\subset\Phi\left(A\right)+\Phi\left(B\right)$$

which can provide possible information about the eigenvalues of $A+B$, given $\Phi\left(A\right)$ and $\Phi\left(B\right)$. In general, given the spectrum $\lambda\left(A\right)$ and $\lambda\left(B\right)$, less can be said about $\lambda\left(A+B\right)$ (see also **art.** 183 and 184). For example, even if the eigenvalues of A and B are known and bounded, the largest eigenvalue of $A+B$ can be unbounded, as deduced from the example inspired by Horn and Johnson (1991, p. 5), where

$$A=\left[\begin{array}{cc} 1-x & 1 \\ f\left(x\right) & x \end{array}\right]\text{ and }B=\left[\begin{array}{cc} 1+x & 1 \\ g\left(x\right) & -x \end{array}\right]$$

Clearly, the eigenvalues of A, B an $A+B$ are

$$\lambda_{1,2}\left(A\right)=\frac{1}{2}\left(1\pm\sqrt{1+4\left(x^{2}-x+f\left(x\right)\right)}\right)$$

$$\lambda_{1,2}\left(B\right)=\frac{1}{2}\left(1\pm\sqrt{1+4\left(x^{2}+x+g\left(x\right)\right)}\right)$$

$$\lambda_{1,2}\left(A+B\right)=\frac{1}{2}\left(1\pm\sqrt{1+4\left(f\left(x\right)+g\left(x\right)\right)}\right)$$

It suffices to choose $f\left(x\right)=-x^{2}+x+c_{1}$ and $g\left(x\right)=-x^{2}-x+c_{2}$ for arbitrary constants c_{1} and c_{2} to have bounded eigenvalues, independent of x, while $\lim_{x\to\infty}\left|\lambda_{1,2}\left(A+B\right)\right|=\infty$.

155. *The spectrum of a unitary matrix.* We denote the eigenvalues of the $n\times n$ unitary matrix U by $\mu_{1},\mu_{2},\ldots,\mu_{n}$.

Theorem 37 *All eigenvalues of a unitary matrix have absolute value 1, i.e., $\left|\mu_{k}\right|=1$ for all $1\leq k\leq n$.*

Proof: The orthogonality relation (8.25) for $k=j$ or the matrix product of the j th diagonal element in I in the orthogonality relation (8.26) equals

$$\sum_{i=1}^{n}\left|U_{ij}\right|^{2}=1$$

which implies that the elements U_{ij} of a unitary matrix cannot exceed unity in absolute value. Therefore, the absolute value of the coefficients c_k in (8.4) of the characteristic polynomial is bounded for any $n \times n$ unitary matrix U. Taking the determinant of the orthogonality relation (8.26) gives

$$1 = \det\left(U^H U\right) = \det\left(U^H\right) \det U = |\det U|^2$$

while (8.6) then leads to $\prod_{k=1}^{n} |\mu_k|^2 = 1$. Hence, a unitary matrix cannot have a zero eigenvalue. In addition, it shows, together with the bounds on $|c_k|$ that are only function of n, that all eigenvalues must lie between some lower and upper bound for any $n \times n$ unitary matrix U and these bounds are not dependent on the unitary matrix elements considered. **Art.** 144 shows that any integer power m (positive as well as negative) of U^m has the same eigenvalues of U raised to the power m. In addition, U^m is also an $n \times n$ orthogonal matrix obeying $(U^m)^H U^m = I$ as follows by induction on

$$(U^m)^H U^m = \left(U^{m-1}\right)^H U^H U U^{m-1} = \left(U^{m-1}\right)^H U^{m-1}$$

Hence, $|\det U^m|^2 = 1$ and, by (8.6), we have, for any $m \in \mathbb{Z}$, that

$$\prod_{k=1}^{n} |\mu_k|^{2m} = 1$$

But, the absolute value of these powers (positive as well as negative) can only remain below a bound independent of m provided $|\mu_k| = 1$ for all k. $\qquad\square$

An orthogonal matrix U_R that obeys $U_R^T U_R = I$ can be regarded as a unitary matrix $U = U_R + iU_I$ with imaginary part $U_I = 0$. In general, an orthogonal matrix is not symmetric, unless $U_R^{-1} = U_R$. Theorem 37 states that the j th eigenvector $z_j = x_j + iy_j$ obeys the eigenvalue equation $U z_j = e^{i\theta_j} z_j$ for real θ_j, explicitly,

$$(U_R + iU_I)(x_j + iy_j) = (\cos\theta_j + i\sin\theta_j)(x_j + iy_j)$$

Thus, in general, the eigenvalues $e^{i\theta_j}$ and eigenvector z_j of an orthogonal matrix U_R (with $U_I = 0$) are complex.

156. *The eigenvalue decomposition of a symmetric (Hermitian) matrix.* **Art.** 151 shows that any real, symmetric matrix $A_{n \times n}$ can be written as $A = X\Lambda X^T$, where $\Lambda = \mathrm{diag}(\lambda_j)_{1 \leq j \leq n}$ and where $X = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}$ is an orthogonal matrix (such that $X^T X = I$) formed by the real and normalized eigenvectors $x_1, x_2, \dots, x_n$ of A corresponding to the eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. In vector notation,

$$A = \sum_{k=1}^{n} \lambda_k x_k x_k^T = \sum_{k=1}^{n} \lambda_k E_k \qquad (8.31)$$

where the matrix $E_k = x_k x_k^T$ is the outer product of x_k by itself. It represents the

orthogonal projection[3] onto the eigenspace of λ_k. For any analytic function f, we have that $f(A) = Xf(\Lambda)X^T$ and

$$f(A) = \sum_{k=1}^{n} f(\lambda_k) E_k \tag{8.32}$$

157. *Properties of the matrix E_k.* From the definition $E_k = x_k x_k^T$, we deduce that $E_k = E_k^T$, thus, symmetric. The explicit form of the matrix E_k is

$$E_k = x_k x_k^T = \begin{bmatrix} (x_{k1})^2 & x_{k1}x_{k2} & x_{k1}x_{k3} & \cdots & x_{k1}x_{kn} \\ x_{k2}x_{k1} & (x_{k2})^2 & x_{k2}x_{k3} & \cdots & x_{k2}x_{kn} \\ x_{k3}x_{k1} & x_{k3}x_{k2} & (x_{k3})^2 & \cdots & x_{k3}x_{kn} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{kn}x_{k1} & x_{kn}x_{k2} & x_{kn}x_{k3} & \cdots & (x_{kn})^2 \end{bmatrix}$$

which shows that the diagonal element $(E_k)_{ii} = (x_{ki})^2$ equals the square of the i th vector component of the eigenvector x_k. Hence,

$$\text{trace}(E_k) = \sum_{i=1}^{n} (x_{ki})^2 = x_k^T x_k = 1 \tag{8.33}$$

It follows from the orthogonality property (8.25) of eigenvectors x_k of a symmetric matrix that $E_k^2 = E_k$ and $E_k E_m = 0$ for $k \neq m$. Let us denote the eigenvalue equation $E_k y_j = \xi_j y_j$ of the symmetric matrix E_k. After left multiplication by E_k, we obtain $E_k^2 y_j = \xi_j^2 y_j$ and, since $E_k^2 = E_k$, we arrive at $E_k y_j = \xi_j^2 y_j$. Hence, for any eigenvalue ξ_j and corresponding eigenvector y_j, we have that $\xi_j y_j = \xi_j^2 y_j$, which implies that ξ_j is either zero or 1. The trace relation (8.7) and (8.33) indicates that $\sum_{j=1}^{n} \xi_j = 1$. Consequently[4], we conclude that $n-1$ eigenvalues are zero and one eigenvalue equals 1, such that $\|E_k\|_2 = 1$, which follows from (8.49). The zero eigenvalues imply that $\det(E_k) = 0$ and that the inverse of E_k does not exist.

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[3] Let $\mathcal{X}$ and $\mathcal{Y}$ be complementary subspaces of a vector space $\mathcal{V}$ so that every vector $v \in \mathcal{V}$ can be uniquely resolved as $v = x + y$, where $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. The unique linear operator P defined by $Pv = x$ is called the projector onto $\mathcal{X}$ along $\mathcal{Y}$ and P has the following properties: (a) $P^2 = P$ (i.e., P is idempotent), (b) $I - P$ is the complementary projector onto $\mathcal{Y}$ along $\mathcal{X}$, (c) If $\mathcal{V}$ is $\mathbb{R}^n$, then

$$P = \begin{bmatrix} X & Y \end{bmatrix} \begin{bmatrix} I & O \\ O & O \end{bmatrix} \begin{bmatrix} X & Y \end{bmatrix}^{-1}$$

where the columns of X and Y are respective bases for $\mathcal{X}$ and $\mathcal{Y}$. These results are proved in Meyer (2000, p. 386). If $\mathcal{Y} = \mathcal{X}^{\perp}$, then P is the orthogonal projector onto $\mathcal{X}$. In that case, Meyer (2000, p. 430) shows that $P = X(X^T X)^{-1} X^T$ and, if the basisvectors of $\mathcal{X}$ are orthogonal, i.e., $X^T X = I$, we have $P = XX^T$.

[4] The eigenvalues of E_k directly follow from the rank-one update formula (8.82) and $x_k^T x_k = 1$ because

$$\det\left(x_k x_x^T - \lambda I\right) = (-\lambda)^n \det\left(I - \frac{1}{\lambda} x_k x_x^T\right) = (-\lambda)^{n-1}(\lambda - 1)$$

Geometrically, this is understood because, by projecting, information is lost and the inverse cannot create information.

The notation so far has implicitly assumed that all eigenvalues are different, which is not the case in general. Thus, if the eigenvalue λ_k has multiplicity m_k, then there are m_k eigenvectors belonging to λ_k that form an orthonormal basis for the eigenspace belonging to λ_k. Let U_k denote the matrix with its columns equal to those m_k eigenvectors belonging to λ_k, then the matrix $E_k = U_k U_k^T$, which is the obvious generalization of $E_k = x_k x_k^T$. Thus, with (8.7), trace(E_k) is equal to the rank of E_k, which is the dimension of the eigenspace associated with λ_k. If the multiplicity of λ_k is m_k, then rank(E_k) $= m_k$.

Consider now the $n \times n$ matrix $Y = \sum_{k=1}^{q} E_k$, where the k index ranges over all distinct $q \le n$ eigenvalues $\{\lambda_k\}_{1 \le k \le q}$ of A. Since $E_k^2 = E_k$ and $E_k E_m = 0$ for $k \ne m$, we find that

$$Y^2 = \sum_{k=1}^{q} E_k \sum_{j=1}^{q} E_j = \sum_{k=1}^{q} E_k^2 + 2 \sum_{k=1}^{q} \sum_{j=1}^{k-1} E_k E_j = Y$$

such that all eigenvalues of the symmetric (Hermitian) matrix Y are either 1 or 0. But,

$$\text{trace}(Y) = \sum_{k=1}^{q} \text{trace}(E_k) = \sum_{k=1}^{q} m_k = n$$

which implies that all eigenvalues of Y must be equal to 1, and thus that $Y = I$. The fact that

$$\sum_{k=1}^{q} E_k = I_{n \times n} \tag{8.34}$$

also follows from (8.32) for $f(x) = e^{zx}$, after letting $z = 0$. Moreover, this relation is rewritten as $XX^T = I$, which, combined with the normalization (8.26), implies that X is an orthogonal matrix, which we already knew from **art. 151**. It means that the sum of the orthogonal projections onto all eigenspaces of A spans again the total $n \times n$ space.

By right multiplying the eigenvalue equation $Ax_k = \lambda_k x_k$ by x_k^T, we obtain

$$AE_k = \lambda_k E_k$$

This result also follows from (8.31) by using the orthogonality property $E_k E_m = E_k 1_{\{k=m\}}$ of the matrices E_k and E_m. Finally, let $f(x) = \frac{c_A(x)}{x - \lambda_k} = \prod_{j=1;j \ne k}^{n} (x - \lambda_j)$, where $c_A(x)$ is the characteristic polynomials of A, then (8.32) shows that

$$\prod_{j=1;j \ne k}^{n} (A - \lambda_j) = f(\lambda_k) E_k$$

Hence, E_k is a polynomial in A.

158.   *Diagonal elements of E_k.*   It directly follows from (8.31) that, for each $1 \leq j \leq n$,

$$a_{jj} = \sum_{k=1}^{n} \lambda_k \left(E_k\right)_{jj} = \sum_{k=1}^{n} \lambda_k \left(x_k\right)_j^2$$

Geometrically, the scalar product of the vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ with the vectors $y_j = \left(x_{1j}^2, x_{2j}^2, \ldots, x_{nj}^2\right)$, where x_{kj} is the j th component of the k th eigenvector of A belonging to λ_k, equals the diagonal element a_{jj}. Denoting the non negative matrix $Y^T = \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix}$ and $b = (a_{11}, a_{22}, \ldots, a_{nn})$, the above relation reads in matrix form

$$Y^T \lambda = b \tag{8.35}$$

Generally, denoting the vector $b_f = \left((f(A))_{11}, (f(A))_{22}, \ldots, (f(A))_{nn}\right)$ and similarly for the vector $\lambda_f = (f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n))$, it follows from (8.32) that

$$Y^T \lambda_f = b_f \tag{8.36}$$

The normalization (8.25) of the eigenvectors shows that the row sum in Y^T is equal to one. Thus,

$$Yu = u$$

which shows that Y and Y^T have an eigenvalue equal to 1 belonging to the eigenvector u. Since Y is a non negative matrix, the Perron Frobenius Theorem in **art.** 168 indicates that this eigenvalue belonging to an eigenvector with non negative components is the largest one and that the absolute value of any other eigenvalue is smaller than 1.

Relation (8.34) translates to

$$1 = \sum_{k=1}^{n} \left(x_k\right)_j^2 \tag{8.37}$$

and to

$$Y^T u = u$$

illustrating that u is both a left and right eigenvector.

Incidentally, Y^T is a doubly stochastic matrix and y_{ij} can be regarded as a transition probability from state j to state i.

159.   *Orthogonal transformation.*   Using the orthogonality property $U^T U = I$, from which $U^{-1} = U^T$, the transformation of a vector z by an orthogonal matrix U results in the vector x such that $x = Uz$ and the inverse transform $z = U^T x$ is also an orthogonal transformation. Moreover, the quadratic form

$$x^T x = z^T U^T U z = z^T z$$

is invariant under an orthogonal transformation. Since $x^T x = \sum_{k=1}^{n} x_k^2$, which can be regarded as the square of the Euclidean distance of the vector x from the

origin, the invariance means that, after orthogonal transformation, that distance is preserved. Geometrically, any orthogonal transformation is a rotation of the vector x around the origin to a vector z, and both x and z have equal Euclidean distance or norm (see **art.** 161).

160. To a real symmetric matrix A, a bilinear form $x^T A y$ is associated, which is a scalar defined as

$$x^T A y = x A y^T = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i y_j$$

We call a bilinear form a quadratic form if $y = x$. A necessary and sufficient condition for a quadratic form to be positive definite, i.e., $x^T A x > 0$ for all $x \neq 0$, is that all eigenvalues of A should be positive. Indeed, **art.** 151 shows the existence of an orthogonal matrix U that transforms A to a diagonal form. Let $x = U z$, then

$$x^T A x = z^T U^T A U z = \sum_{k=1}^{n} \lambda_k z_k^2 \qquad (8.38)$$

which is only positive for all z_k provided $\lambda_k > 0$ for all k. From (8.6), a positive definite quadratic form $x^T A x$ possesses a positive determinant, $\det A > 0$. This analysis shows that the problem of determining an orthogonal matrix U (or the eigenvectors of A) is equivalent to the geometrical problem of determining the principal axes of the hyper ellipsoid

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i y_j = 1$$

Relation (8.38) illustrates that the eigenvalue λ_k^{-1} is the square of the principal axis along the z_k vector. A multiple eigenvalue refers to an indeterminacy of the principal axes. For example if $n = 3$, an ellipsoid with two equal principal axis means that any section along the third axis is a circle. Any two perpendicular diameters of the largest circle orthogonal to the third axis are principal axes of that ellipsoid.

For additional properties of quadratic forms, such as the inertial theorem[5], we refer to Courant and Hilbert (1953) and Gantmacher (1959a).

8.4 Vector and matrix norms

161. Vector and matrix norms, denoted by $\|x\|$ and $\|A\|$ respectively, provide a single number reflecting a "size" of the vector or matrix and may be regarded as an extension of the concept of the modulus of a complex number. A norm is a certain

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[5] The inertial theorem states that the number of positive and negative coefficients in a quadratic form reduced to the form (8.38) by a nonsigular real linear transformation does not depend on the particular transformation.

function of the vector components or matrix elements. All norms, vector as well as matrix norms, satisfy the three "distance" relations:

(i) $\|x\| > 0$ unless $x = 0$;
(ii) $\|\alpha x\| = |\alpha| \, \|x\|$ for any complex number α;
(iii) $\|x + y\| \le \|x\| + \|y\|$

In general, the Hölder q norm of a vector x is defined as

$$\|x\|_q = \left(\sum_{j=1}^{n} |x_j|^q \right)^{1/q} \tag{8.39}$$

For example, the well known Euclidean norm or length of the vector x is found for $q = 2$ and $\|x\|_2^2 = x^H x$. In probability theory where x denotes a discrete probability density function, the law of total probability states that $\|x\|_1 = \sum_{j=1}^{n} x_j = 1$ and we will write $\|x\|_1 = \|x\|$. Finally, $\max |x_j| = \lim_{q \to \infty} \|x\|_q = \|x\|_\infty$. The unit spheres $S_q = \{x \mid \|x\|_q = 1\}$ are, in three dimensions $n = 3$, for $q = 1$ an octahedron; for $q = 2$ a ball; and for $q = \infty$ a cube. Furthermore, S_1 fits into S_2, which in turn fits into S_∞, and this implies that $\|x\|_1 \ge \|x\|_2 \ge \|x\|_\infty$ for any x.

The Hölder inequality states that, for $\frac{1}{p} + \frac{1}{q} = 1$ and real $p, q > 1$,

$$\left| x^H y \right| \le \|x\|_p \, \|y\|_q \tag{8.40}$$

and is given explicitly in (9.46). A special case of the Hölder inequality where $p = q = 2$ is the Cauchy Schwarz inequality

$$\left| x^H y \right| \le \|x\|_2 \, \|y\|_2 \tag{8.41}$$

The Cauchy Schwarz inequality (8.41) follows immediately from the Cauchy identity (8.86) as shown in **art.** 192. The $q = 2$ norm is invariant under a unitary (hence also orthogonal) transformation U, where $U^H U = I$, because $\|Ux\|_2^2 = x^H U^H U x = x^H x = \|x\|_2^2$ (see **art.** 159).

Another example of a non homogeneous vector norm is the quadratic form

$$\sqrt{\|x\|_A} = \sqrt{x^T A x}$$

provided A is positive definite. Relation (8.38) shows that, if not all eigenvalues λ_j of A are the same, then not all components of the vector x are weighted similarly and, thus, in general, $\sqrt{\|x\|_A}$ is a non homogeneous norm. The quadratic form $\|x\|_I$ equals the homogeneous Euclidean norm $\|x\|_2^2$.

8.4.1 Properties of norms

162. All norms are equivalent in the sense that there exist positive real numbers c_1 and c_2 such that, for all x,

$$c_1 \|x\|_p \le \|x\|_q \le c_2 \|x\|_p$$

For example,

$$\|x\|_2 \le \|x\|_1 \le \sqrt{n}\,\|x\|_2$$
$$\|x\|_\infty \le \|x\|_1 \le n\,\|x\|_\infty$$
$$\|x\|_\infty \le \|x\|_2 \le \sqrt{n}\,\|x\|_\infty$$

By choosing in the Hölder inequality $p = q = 1$, $x_j \to \alpha_j x_j^s$ for real $s > 0$ and $y_j \to \alpha_j > 0$, we obtain with $0 < \theta < 1$ an inequality for the *weighted q* norm

$$\left(\frac{\sum_{j=1}^{n} \alpha_j |x_j|^{s\theta}}{\sum_{j=1}^{n} \alpha_j} \right)^{\frac{1}{s\theta}} \le \left(\frac{\sum_{j=1}^{n} \alpha_j |x_j^s|}{\sum_{j=1}^{n} \alpha_j} \right)^{\frac{1}{s}}$$

For $\alpha_j = 1$, the weights α_j disappear such that the inequality for the Hölder q norm becomes

$$\|x\|_{s\theta} \le \|x\|_s\, n^{\frac{1}{s}(\frac{1}{\theta} - 1)}$$

where $n^{\frac{1}{s}(\frac{1}{\theta}-1)} \ge 1$. On the other hand, with $0 < \theta < 1$ and for real $s > 0$,

$$\frac{\|x\|_s}{\|x\|_{s\theta}} = \frac{\left(\sum_{j=1}^{n} |x_j|^s \right)^{\frac{1}{s}}}{\left(\sum_{k=1}^{n} |x_k|^{s\theta} \right)^{\frac{1}{s\theta}}} = \left(\sum_{j=1}^{n} \frac{|x_j|^s}{\left(\sum_{k=1}^{n} |x_k|^{s\theta} \right)^{\frac{1}{\theta}}} \right)^{\frac{1}{s}} = \left(\sum_{j=1}^{n} \left(\frac{|x_j|^{s\theta}}{\sum_{k=1}^{n} |x_k|^{s\theta}} \right)^{\frac{1}{\theta}} \right)^{\frac{1}{s}}$$

Since $y = \frac{|x_j|^{s\theta}}{\sum_{k=1}^{n} |x_k|^{s\theta}} \le 1$ and $\frac{1}{\theta} > 1$, it holds that $y^{\frac{1}{\theta}} \le y$ and

$$\left(\sum_{j=1}^{n} \left(\frac{|x_j|^{s\theta}}{\sum_{k=1}^{n} |x_k|^{s\theta}} \right)^{\frac{1}{\theta}} \right)^{\frac{1}{s}} \le \left(\sum_{j=1}^{n} \frac{|x_j|^{s\theta}}{\sum_{k=1}^{n} |x_k|^{s\theta}} \right)^{\frac{1}{s}} = \left(\frac{\sum_{j=1}^{n} |x_j|^{s\theta}}{\sum_{k=1}^{n} |x_k|^{s\theta}} \right)^{\frac{1}{s}} = 1$$

which leads to an opposite inequality,

$$\|x\|_s \le \|x\|_{s\theta}$$

In summary, if $p > q > 0$, then the general inequality for Hölder q norm is

$$\|x\|_p \le \|x\|_q \le \|x\|_p\, n^{\frac{1}{q} - \frac{1}{p}} \tag{8.42}$$

163. For $m \times n$ matrices A, the most frequently used norms are the Euclidean or Frobenius norm

$$\|A\|_F = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2} \tag{8.43}$$

and the q norm

$$\|A\|_q = \sup_{x \ne 0} \frac{\|Ax\|_q}{\|x\|_q} \tag{8.44}$$

The second distance relation in **art. 161**, $\frac{\|Ax\|_q}{\|x\|_q} = \left\| A \frac{x}{\|x\|_q} \right\|_q$, shows that

$$\|A\|_q = \sup_{\|x\|_q = 1} \|Ax\|_q \tag{8.45}$$

Furthermore, the matrix q norm (8.44) implies that

$$\|Ax\|_q \le \|A\|_q \|x\|_q \tag{8.46}$$

Since the vector norm is a continuous function of the vector components and since the domain $\|x\|_q = 1$ is closed, there must exist a vector x for which equality $\|Ax\|_q = \|A\|_q \|x\|_q$ holds. Since the k th vector component of Ax is $(Ax)_i = \sum_{j=1}^n a_{ij} x_j$, it follows from (8.39) that

$$\|Ax\|_q = \left(\sum_{i=1}^m \left| \sum_{j=1}^n a_{ij} x_j \right|^q \right)^{1/q}$$

For example, for all x with $\|x\|_1 = 1$, we have that

$$\|Ax\|_1 = \sum_{i=1}^m \left| \sum_{j=1}^n a_{ij} x_j \right| \le \sum_{i=1}^m \sum_{j=1}^n |a_{ij}|\,|x_j| = \sum_{j=1}^n |x_j| \sum_{i=1}^m |a_{ij}|$$

$$\le \sum_{j=1}^n |x_j| \left(\max_j \sum_{i=1}^m |a_{ij}| \right) = \max_j \sum_{i=1}^m |a_{ij}|$$

Clearly, there exists a vector x for which equality holds, namely, if k is the column in A with maximum absolute sum, then $x = e_k$, the k th basis vector with all components zero, except for the k th one, which is 1. Similarly, for all x with $\|x\|_\infty = 1$,

$$\|Ax\|_\infty = \max_i \left| \sum_{j=1}^n a_{ij} x_j \right| \le \max_i \sum_{j=1}^n |a_{ij}|\,|x_j| \le \max_i \sum_{j=1}^n |a_{ij}|$$

Again, if r is the row with maximum absolute sum and $x_j = 1.\text{sign}(a_{rj})$ such that $\|x\|_\infty = 1$, then $(Ax)_r = \sum_{j=1}^n |a_{rj}| = \max_i \sum_{j=1}^n |a_{ij}| = \|Ax\|_\infty$. Hence, we have proved that

$$\|A\|_\infty = \max_i \sum_{j=1}^n |a_{ij}| \tag{8.47}$$

$$\|A\|_1 = \max_j \sum_{i=1}^m |a_{ij}| \tag{8.48}$$

from which

$$\left\| A^H \right\|_\infty = \|A\|_1$$

164. The $q = 2$ matrix norm, $\|Ax\|_2$, is obtained differently. Consider

$$\|Ax\|_2^2 = (Ax)^H Ax = x^H A^H Ax$$

Since $A^H A$ is a Hermitian matrix, **art.** 151 shows that all eigenvalues are real and non negative because a norm $\|Ax\|_2^2 \ge 0$. These ordered eigenvalues are denoted as

$\sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_n^2 \geq 0$. Applying the theorem in **art.** 151, there exists a unitary matrix U such that $x = Uz$ yields

$$x^H A^H A x = z^H U^H A^H A U z = z^H \text{diag}\left(\sigma_j^2\right) z \leq \sigma_1^2 z^H z = \sigma_1^2 \|z\|_2^2$$

Since the $q = 2$ norm is invariant under a unitary (orthogonal) transform $\|x\|_2 = \|z\|_2$, by the definition (8.44),

$$\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_1 \qquad (8.49)$$

where the supremum is achieved if x is the eigenvector of $A^H A$ belonging to σ_1^2. Meyer (2000, p. 279) proves the corresponding result for the minimum eigenvalue provided that A is non singular,

$$\left\|A^{-1}\right\|_2 = \frac{1}{\min_{\|x\|_2=1} \|Ax\|_2} = \sigma_n^{-1}$$

The non negative quantity σ_j is called the j th singular value and σ_1 is the largest singular value of A. The importance of this result lies in an extension of the eigenvalue problem to non square matrices, which is called the singular value de composition. A detailed discussion is found in Golub and Van Loan (1996) and Horn and Johnson (1991, Chapter 3).

165. The Frobenius norm $\|A\|_F^2 = \text{trace}\left(A^H A\right)$. With (8.7) and the analysis of $A^H A$ above,

$$\|A\|_F^2 = \sum_{k=1}^{n} \sigma_k^2 \qquad (8.50)$$

In view of (8.49), the bounds $\|A\|_2 \leq \|A\|_F \leq \sqrt{n}\,\|A\|_2$ may be attained.

8.4.2 Applications of norms

166. (a) Since $\left\|A^k\right\| = \left\|AA^{k-1}\right\| \leq \|A\| \left\|A^{k-1}\right\|$, by induction, we have for any integer k, that

$$\left\|A^k\right\| \leq \|A\|^k$$

and

$$\lim_{k \to \infty} A^k = 0 \text{ if } \|A\| < 1$$

(b) By taking the norm of the eigenvalue equation (8.1), $\|Ax\| = |\lambda|\,\|x\|$ and with (8.46),

$$|\lambda| \leq \|A\|_q \qquad (8.51)$$

Applied to $A^H A$, for any q norm,

$$\sigma_1^2 \leq \left\|A^H A\right\|_q \leq \left\|A^H\right\|_q \|A\|_q$$

Choose $q = 1$ and with (8.49),

$$\|A\|_2^2 \leq \left\|A^H\right\|_1 \|A\|_1 = \|A\|_\infty \|A\|_1$$

(c) Any matrix A can be transformed by a similarity transform H to a Jordan canonical form C (art. **4**) as $A = HCH^{-1}$, from which $A^k = HC^kH^{-1}$. A typical Jordan submatrix $(C_m(\lambda))^k = \lambda^{k-2}B$, where B is independent of k. Hence, for large k, $A^k \to 0$ if and only if $|\lambda| < 1$ for all eigenvalues.

8.5 Non-negative matrices

167. *Reducibility.* A matrix A is reducible if there is a relabeling that leads to

$$\widetilde{A} = \left[\begin{array}{cc} A_1 & B \\ O & A_2 \end{array} \right]$$

where A_1 and A_2 are square matrices. Otherwise A is irreducible. Relabeling amounts to permuting rows and columns in the same fashion. Thus, there exists a similarity transform H such that $A = H\widetilde{A}H^{-1}$. For doubly stochastic matrices, where $\sum_{k=1}^n a_{kj} = \sum_{k=1}^n a_{jk} = 1$, Fiedler (1972) has proposed the "measure $r(A)$ of irreducibility" of A defined as

$$r(A) = \min_{\mathcal{M} \subset \mathcal{N}} \sum_{i \in \mathcal{M}, k \notin \mathcal{M}} a_{ik} \tag{8.52}$$

because A is reducible if there exists a non empty subset $\mathcal{M}$ of the set of all indices (or nodes) $\mathcal{N}$ such that $a_{ik} = 0$ for all $i \in \mathcal{M}$ and $k \notin \mathcal{M}$. Hence, if A is reducible, then $r(A) = 0$. Since $\sum_{i \in \mathcal{M}, k \notin \mathcal{M}} a_{ik} \leq \sum_{k=2}^n a_{1k} \leq 1$, the measure of irreducibility lies between $0 \leq r(A) \leq 1$.

168. *The famous Perron Frobenius theorem for non negative matrices.*

Theorem 38 (Perron-Frobenius) *An irreducible non negative $n \times n$ matrix A always has a real, positive eigenvalue $\lambda_1 = \lambda_{\max}(A)$ and the modulus of any other eigenvalue does not exceed $\lambda_{\max}(A)$, i.e., $|\lambda_k(A)| \leq \lambda_{\max}(A)$ for $k = 2, \ldots, n$. Moreover, λ_1 is a simple zero of the characteristic polynomial $\det(A - \lambda I)$. The eigenvector belonging to λ_1 has positive components.*

If A has h eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_h$ with $|\lambda_h| = \lambda_1$, then all these equal moduli eigenvalues satisfy the polynomial $\lambda^h - \lambda_1^h = 0$, i.e., $\lambda_k = \lambda_1 e^{\frac{2\pi i(k-1)}{h}}$ for $k = 1, \ldots, h$.

Proof: See, e.g., Gantmacher (1959b, Chapter XIII). $\qquad\qquad\square$

If a non negative $n \times n$ matrix A is reducible, then A has always a *non negative* eigenvalue $\lambda_{\max}(A)$ and no other eigenvalue has a larger modulus than $\lambda_{\max}(A)$. The corresponding eigenvector belonging to $\lambda_{\max}(A)$ has *non negative* components. Hence, reducibility removes the positivity of the largest eigenvalue and that of the

components of its corresponding eigenvector. An essential Lemma in Frobenius'
proof, beside the variational property of the largest eigenvalue

$$\lambda_{\max}(A) = \max_{x \neq 0} \min_{1 \leq j \leq n} \frac{(Ax)_j}{x_j} \tag{8.53}$$

akin to Rayleigh's inequality (8.28) and a consequence of (8.54) in **art. 169** for a
symmetric matrix, is:

Lemma 6 *If A is a $n \times n$ non negative, irreducible matrix and C is an $n \times n$ complex
matrix, in which each element obeys $|c_{ij}| \leq a_{ij}$, then every eigenvalue $\lambda(C)$ of C
satisfies the inequality $|\lambda(C)| \leq \lambda_{\max}(A)$.*

   Proof: See, e.g., Gantmacher (1959b, Chapter XIII).   □

   An application of Lemma 6 is the following lemma for non negative matrices,
which is useful in assessing the largest eigenvalue of the adjacency matrix of a
graph:

Lemma 7 *If one element in a non negative matrix A is increased, then the largest
eigenvalue is also increased. The increase is strict for irreducible matrices.*

   Proof: Consider the non negative matrix C and $A = C + \varepsilon e_i e_j^T$, where $\varepsilon > 0$,
e_i and e_j are the basic vectors and $\widetilde{O} = e_i e_j^T$ is the zero matrix, except for the
element $\widetilde{O}_{ij} = 1$. Lemma 6 shows that $\lambda_{\max}(A) \geq \lambda(C)$. We now demonstrate the
strict inequality for irreducible matrices. If x denotes the eigenvector belonging to
the largest eigenvalue of C, then the variational property (8.53) implies

$$\lambda_{\max}(A) \geq \frac{x^T A x}{x^T x} = \frac{x^T C x}{x^T x} + \varepsilon \frac{x^T e_i e_j^T x}{x^T x}$$
$$= \lambda_{\max}(C) + \varepsilon \frac{x_i x_j}{x^T x}$$

Since all components of the largest eigenvector x are non negative (and even positive
if C is irreducible), the lemma is proved.   □

169. *Bounds for the largest eigenvalue of symmetric, irreducible, non negative ma
trices.* If the irreducible, non negative matrix is symmetric, we can exploit symme
try to deduce bounds for the largest eigenvalue by considering the quadratic form
$y^T A x_1 = x_1^T A y$, where x_1 is the eigenvector with positive components (Perron
Frobenius Theorem 38) belonging to the largest eigenvalue λ_1 and y is a vector
with positive components. Using the eigenvalue equation $A x_1 = \lambda_1 x_1$, we obtain
$y^T A x_1 = \lambda_1 y^T x_1$. On the other hand, we have

$$x_1^T A y = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} (x_1)_i y_j = \sum_{i=1}^{N} (x_1)_i y_i \left(\sum_{j=1}^{N} \frac{a_{ij} y_j}{y_i} \right)$$

and, since the components of y and x_1 are positive,

$$\left(\min_{1 \le i \le N} \sum_{j=1}^{N} \frac{a_{ij} y_j}{y_i} \right) \sum_{i=1}^{N} (x_1)_i \, y_i \le x_1^T A y \le \left(\max_{1 \le i \le N} \sum_{j=1}^{N} \frac{a_{ij} y_j}{y_i} \right) \sum_{i=1}^{N} (x_1)_i \, y_i$$

By combining both expressions, taking into account that $y^T x_1 = \sum_{i=1}^{N} (x_1)_i \, y_i > 0$, we obtain the bounds

$$\min_{1 \le i \le N} \frac{(Ay)_i}{y_i} \le \lambda_1 \le \max_{1 \le i \le N} \frac{(Ay)_i}{y_i} \tag{8.54}$$

which are valid for any symmetric, irreducible, non negative matrix A.

170. The next remarkable theorem by Fiedler (1972) bounds the spectral gap for symmetric stochastic matrices.

Theorem 39 (Fiedler) *Let P be a symmetric stochastic $n \times n$ matrix with second largest eigenvalue $\lambda_2(P)$. Then*

$$\psi_n(r(P)) \le 1 - \lambda_2(P) \le \frac{n}{n-1} r(P) \tag{8.55}$$

where the measure of irreducibility $r(A)$ is defined in (8.52) and where the continuous, convex and increasing function $\psi_n(x) \in [0,1]$ is

$$\psi_n(x) = \begin{cases} 2x\left(1 - \cos \frac{\pi}{n}\right) & 0 \le x \le \frac{1}{2} \\ 1 - 2(1-x)\cos \frac{\pi}{n} - (2x-1)\cos \frac{2\pi}{n} & \frac{1}{2} < x \le 1 \end{cases}$$

The inequality (8.55) is best possible: if $u, v \in \mathbb{R}$ satisfy $0 \le u \le 1$ and $\psi_n(u) \le 1 - v \le \frac{n}{n-1} u$, then there exists a symmetric stochastic matrix P with $r(P) = u$ and $\lambda_2(P) = v$.

Proof: The proof is rather involved and we refer to Fiedler (1972). □

171. *Eigenvector components of a non negative matrix.* Fiedler (1975) found a nice property regarding the signs of eigenvector components of a non negative symmetric matrix, that have a profound impact on graph partitioning (**art.** 103).

Theorem 40 (Fiedler) *Let A be an irreducible, non negative symmetric $n \times n$ matrix with eigenvalues $\lambda_1(A) \ge \lambda_2(A) \ge \ldots \lambda_n(A)$ and z be a vector such that $Az \ge \lambda_k(A) z$ with $k \ge 2$. Then, the set of indices (nodes) $\mathcal{M} = \{j \in \mathcal{N} : z_j \ge 0\}$ is not empty and the number of connected components of the principal submatrix $A(\mathcal{M})$, with indices of rows and columns belonging to $\mathcal{M}$, is not larger than $k-1$.*

Before proving the theorem, we rephrase the theorem when A is the adjacency matrix of a graph G. The non negative vector components of z correspond to nodes, that induce a subgraph, specified by the adjacency matrix $A(\mathcal{M})$, with at most $k-1$ distinct connected components.

Proof[6]: The set $\mathcal{M}$ cannot be empty. For, if $\mathcal{M}$ were empty, then all components of z would be negative such that $v = -z$ satisfies $Av \leq \lambda_k(A)v$. Since A is irreducible, Perron Frobenius Theorem 38 demonstrates that $Ax_1 = \lambda_1(A)x_1$ and $\lambda_1(A) > \max(\lambda_2(A), \lambda_n(A))$. Thus,

$$x_1^T Av = \lambda_1(A)x_1^T v > \lambda_k(A)x_1^T v$$

while the hypothesis implies that $x_1^T Av \leq \lambda_k(A)x_1^T v$, which leads to a contradiction. If $\mathcal{M} = \mathcal{N}$, the theorem is true by the Perron Frobenius Theorem 38. Suppose now that $\mathcal{M} \neq \mathcal{N}$. Then, we can always write the matrix A as

$$A = \begin{bmatrix} \widetilde{A} & C \\ C^T & D \end{bmatrix}$$

where $\widetilde{A}$ consists of r distinct connected or irreducible matrices A_j, subject to

$$\sum_{j=1}^{r} \dim(A_j) = \dim \mathcal{M} < n$$

with structure

$$\widetilde{A} = \begin{bmatrix} A_1 & O & \cdots & O \\ O & A_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & O \\ O & \cdots & O & A_r \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_r \end{bmatrix}$$

We partition the vector z conformally,

$$z = \begin{bmatrix} x \\ -y \end{bmatrix}$$

where the vector $x^T = \begin{bmatrix} x_1^T & x_2^T & \cdots & x_r^T \end{bmatrix}$ has subvectors x_j all with non negative components whose indices belong to $\mathcal{M}$. This implies that y contains only positive components, otherwise a component of y would belong to $\mathcal{M}$. The condition $Az \geq \lambda_k(A)z$ implies that $A_j x_j - C_j y \geq \lambda_k(A)x_j$. Since A is irreducible, none of the block matrices C_j can be zero such that $C_j y \geq 0$, with inequality in some component because all components of y are strictly positive. Hence, $A_j x_j \geq \lambda_k(A)x_j$ holds with strict inequality in some component which implies that, for $1 \leq j \leq r$,

$$x_j^T A_j x_j > \lambda_k(A)x_j^T x_j$$

By construction, each A_j is irreducible. The Perron Frobenius Theorem 38 and the Rayleigh inequality (**art.** 152) for the largest eigenvalue state that $\lambda_1(A_j)x_j^T x_j \geq x_j^T A_j x_j$ such that $\lambda_1(A_j) > \lambda_k(A)$. Finally, the interlacing Theorem 42 shows that, if $\lambda_1(A_j) > \lambda_k(A)$ for all $1 \leq j \leq r$, then $\lambda_r(A) > \lambda_k(A)$ and $r \leq k - 1$. This proves the theorem. $\square$

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[6] We have combined Fiedler's proof with that of Powers (1988).

An immediate consequence is that the vector $z = \alpha v_1 + v_2$, where v_1 is the largest eigenvector (with all positive components) and v_2 is the second largest eigenvector of A, satisfies, for $\alpha \geq 0$,

$$A(\alpha v_1 + v_2) = \alpha \lambda_1(A) v_1 + \lambda_2(A) v_2 \geq \lambda_2(A)(\alpha v_1 + v_2)$$

and thus the inequality in Theorem 40 for $k = 2$. Hence, the index set $\mathcal{M} = \left\{ j \in \mathcal{N} : \alpha(v_1)_j + (v_2)_j \geq 0 \right\}$ corresponds to an irreducible submatrix of $A(\mathcal{M})$. Since A and $A(\mathcal{M})$ are irreducible, it means that $A(\mathcal{M}^c)$, where $\mathcal{M} \cup \mathcal{M}^c = \mathcal{N}$ and $\mathcal{M}^c = \left\{ j \in \mathcal{N} : \alpha(v_1)_j + (v_2)_j < 0 \right\}$, is also irreducible. This index set $\mathcal{M}$ decomposes the set of indices (nodes) into two irreducible submatrices (connected subgraphs).

172. *Bounds on eigenvalues of symmetric, non negative and irreducible matrices.* We present a consequence of Fiedler's eigenvector component Theorem 40. We consider the eigenvalue equation $Ax_k = \lambda_k(A) x_k$, where the eigenvalue $\lambda_k(A)$ is smaller than the largest eigenvalue $\lambda_1(A)$. The corresponding real eigenvector x_k is orthogonal to x_1, whose vectors components are positive by virtue of the Perron Frobenius Theorem 38. Let us denote the nodal sets

$$\mathcal{M}_+ = \left\{ j \in \mathcal{N} : (x_k)_j > 0 \right\}, \mathcal{M}_- = \left\{ j \in \mathcal{N} : (x_k)_j < 0 \right\}, \mathcal{M}_0 = \left\{ j \in \mathcal{N} : (x_k)_j = 0 \right\}$$

such that $\mathcal{M}_+ \cup \mathcal{M}_- \cup \mathcal{M}_0 = \mathcal{N}$. Since $x_k^T x_1 = 0$ (by orthogonality, **art. 151**), it holds that $|\mathcal{M}_+| \geq 1$ and $|\mathcal{M}_-| \geq 1$, whence $|\mathcal{M}_0| \leq N - 2$ for any eigenvalue $\lambda_k(A)$ with index $k > 1$.

Suppose that $(x_k)_l = \min_{1 \leq j \leq N} (x_k)_j < 0$ and $(x_k)_m = \max_{1 \leq j \leq N} (x_k)_j > 0$. The eigenvalue equation (1.3) for component l is, assuming that $\lambda_k(A) > 0$,

$$\lambda_k(A)(x_k)_l = \sum_{j=1}^{N} a_{lj}(x_k)_j \geq (|\mathcal{M}_-| - 1)(x_k)_l$$

while that for component m is

$$\lambda_k(A)(x_k)_m \leq (|\mathcal{M}_+| - 1)(x_k)_m$$

Thus, provided $\lambda_k(A) > 0$, we have that $\lambda_k(A) \leq (|\mathcal{M}_-| - 1)$ and $\lambda_k(A) \leq (|\mathcal{M}_+| - 1)$, from which

$$\lambda_k(A) \leq \min(|\mathcal{M}_-|, |\mathcal{M}_+|) - 1 \leq \frac{|\mathcal{M}_-| + |\mathcal{M}_+|}{2} - 1 = \frac{N - |\mathcal{M}_0|}{2} - 1$$

Since $|\mathcal{M}_0| \geq 0$, we find that

$$\lambda_2(A) \leq \left\lfloor \frac{N}{2} \right\rfloor - 1 \tag{8.56}$$

When $\lambda_k(A) < 0$, we obtain similarly

$$\lambda_k(A)(x_k)_l = |\lambda_k(A)| \cdot |(x_k)_l| \leq |\mathcal{M}_+| (x_k)_m$$

and

$$\lambda_k\left(A\right)\left(x_k\right)_m \geq |\mathcal{M}_-|\left(x_k\right)_l$$

or

$$|\lambda_k\left(A\right)|\left(x_k\right)_m \leq |\mathcal{M}_-|\left(x_k\right)_l$$

from which we deduce, after multiplying both inequalities

$$|\lambda_k\left(A\right)| \leq \sqrt{|\mathcal{M}_+||\mathcal{M}_-|} \leq \frac{|\mathcal{M}_-| + |\mathcal{M}_+|}{2}$$

Since $\sqrt{|\mathcal{M}_+||\mathcal{M}_-|} = \sqrt{|\mathcal{M}_+|\left(N - |\mathcal{M}_+| - |\mathcal{M}_0|\right)}$ and $|\mathcal{M}_0| \geq 0$, this quantity is maximal if $|\mathcal{M}_+| = \left\lfloor \frac{N}{2} \right\rfloor$ and $|\mathcal{M}_0| = 0$. Hence, the smallest eigenvalue of A obeys

$$\lambda_N\left(A\right) \geq -\sqrt{\left\lfloor \frac{N}{2} \right\rfloor \left\lceil \frac{N}{2} \right\rceil} \tag{8.57}$$

In addition to this bound (8.57), the Perron Frobenius Theorem 38 as well as Theorem 63 indicate that $\lambda_N\left(A\right) \geq -\lambda_1\left(A\right)$.

We end this section on non negative matrices by pointing to yet another nice article by Fiedler and Pták (1962), that studies the class of real square matrices with non positive off diagonal elements, to which the Laplacian matrix of a graph belongs. We also mention *totally positive matrices*. An $n \times m$ matrix is said to be totally positive if all its minors are non negative. The current state of the art is treated by Pinkus (2010), who shows that the eigenvalues of square, totally positive matrices are both real and non negative.

8.6 Positive (semi) definiteness

173. *Positive definiteness.* A matrix $A \in \mathbb{R}^{n \times n}$ is positive definite if the quadratic form $x^T A x > 0$ for all non zero vectors $x \in \mathbb{R}^n$. This definition implies that A is nonsingular for otherwise there would exist a non zero vector x such that $x^T A x = 0$.

We start with a *basic property*: If $A \in \mathbb{R}^{n \times n}$ is positive definite and $Y \in \mathbb{R}^{k \times n}$ has rank k, then the $k \times k$ matrix $B = Y^T A Y$ is also positive definite. Indeed, suppose that the non zero vector $z \in \mathbb{R}^k$ satisfies $0 \geq z^T B z = \left(Yz\right)^T A Y z$, then $Yz = 0$ by the positive definiteness of A. But Y has full column rank, which implies that $z = 0$, leading to a contradiction.

A consequence of the basic property is that all principal submatrices of A are positive definite. In particular, *all diagonal elements of a positive definite matrix A are positive*. By choosing Y equal to the k column vectors of the identity matrix $I_{n \times n}$, any principal submatrix of A is found as $B = Y^T A Y$. The basic property then demonstrates the consequence.

If A is positive semidefinite, then any principal submatrix of A is also positive semidefinite. This property is less stringent than the basic property for positive definiteness, because $z^T B z = \left(Yz\right)^T A Y z \geq 0$ for any vector Yz.

174. *Elements in a symmetric positive semidefinite matrix.* If $A \in \mathbb{R}^{n \times n}$ is sym metric positive semidefinite, then

$$|a_{ij}| \leq \frac{1}{2} (a_{ii} + a_{jj}) \tag{8.58}$$

$$|a_{ij}| \leq \sqrt{a_{ii}a_{jj}} \tag{8.59}$$

Proof: We first show the arithmetic mean inequality (8.58). Positive semi definiteness implies that $x^T A x \geq 0$ for any vector x. Choose now $x = e_i + e_j$, where e_i is a basis vector with all components zero except at position i where it is one. Then, $x^T A x = a_{ii} + a_{jj} + 2a_{ij} \geq 0$. Similarly, for $x = e_i - e_j$, we find $x^T A x = a_{ii} + a_{jj} - 2a_{ij} \geq 0$. Combining both inequalities demonstrates the arithmetic mean inequality. Since the inequality holds for all i and j, it also implies

$$\max_{i,j} |a_{ij}| \leq \max_j a_{jj}$$

The geometric mean inequality (8.59) follows by considering a principal submatrix of A, which is also positive semidefinite (**art. 173**). Without loss of generality, we can choose the principal submatrix $A_s = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ and the vector $z = \begin{bmatrix} x \\ 1 \end{bmatrix}$. Then, $0 \leq z^T A_s z = a_{11}x^2 + 2a_{12}x + a_{22}$, which requires that the discriminant $4a_{12}^2 - 4a_{11}a_{22} \leq 0$. $\qquad\square$

175. The *Gram matrix* associated to the vectors $a_1, a_2, \ldots, a_n$ is defined as

$$G = A^T A, \qquad A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

so that $G_{ij} = a_i^T a_j$ and $G_{ii} = a_i^T a_i = |a_i|^2$ for $i = 1, \ldots, n$. The Gram matrix $G = A^T A$ is symmetric and positive semidefinite because $x^T G x = (Ax)^T A x = \|Ax\|_2^2 \geq 0$. **Art.** 160 implies that all eigenvalues of G are real and non negative. When a matrix G is positive semidefinite and symmetric, we can find the ma trix A as the square root $A = \sqrt{G}$. Indeed, the eigenvalue decomposition is $G = U \text{diag}(\lambda_k(G)) U^T$, where $U = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}$ is an orthogonal ma trix $(U^T U = UU^T = I)$ formed by the scaled, real eigenvectors u_k belonging to eigenvalue $\lambda_k(G)$. Since all eigenvalues are real and non negative, it holds that $\sqrt{\lambda_k(G)}$ are real such that

$$G = U \text{diag}(\lambda_k(G)) U^T = U \text{diag}\left(\sqrt{\lambda_k(G)}\right) \text{diag}\left(\sqrt{\lambda_k(G)}\right) U^T$$

$$= U \text{diag}\left(\sqrt{\lambda_k(G)}\right) \left(U \text{diag}\left(\sqrt{\lambda_k(G)}\right)\right)^T$$

Hence, we can find the matrix $A = \text{diag}\left(\sqrt{\lambda_k(G)}\right) U^T$, which is symmetric[7].

Moreover, if R is an orthogonal matrix for which $R^T R = I$, then $\tilde{A} = RA$ has a

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[7] The Cholesky method gives a solution $A \quad \sqrt{G}$ that is, in general, not symmetric. Another example of a non-symmetric "square root" matrix A is given in **art.** 264.

same Gram matrix since

$$\tilde{G} = \tilde{A}^T \tilde{A} = (RA)^T RA = A^T R^T RA = A^T A = G$$

Hence, given a solution A of $G = A^T A$, all other solutions are found by orthogonal transformation.

In summary, any symmetric, positive semidefinite matrix can be considered as a Gram matrix G whose diagonal elements are non negative, $G_{ii} \geq 0$. The non negativeness of the diagonal elements was already demonstrated in **art.** 173 and **art.** 174.

176. If all eigenvalues are real and $\lambda_k \geq 0$ as in a symmetric, positive semidefinite matrix (**art.** 160), we can apply the general theorem of the arithmetic and geometric mean in several real variables $x_k \geq 0$, which is nicely treated by Hardy *et al.* (1999),

$$\prod_{k=1}^{n} x_k^{q_k} \leq \sum_{k=1}^{n} q_k x_k \tag{8.60}$$

where $\sum_{k=1}^{n} q_k = 1$, to (8.6) and (8.7) with $q_k = \frac{\alpha_k}{\sum_j^n {}_1 \alpha_j} \geq 0$,

$$\prod_{k=1}^{n} \lambda_k^{\alpha_k} \leq \left(\frac{\sum_{k=1}^{n} \alpha_k \lambda_k}{\sum_{j=1}^{n} \alpha_j} \right)^{\sum_j^n {}_1 \alpha_j}$$

By choosing $\alpha_j = 1$, we find the inequality

$$\det A \leq \left(\frac{\text{trace}(A)}{n} \right)^n$$

177. Let M be a symmetric and positive semidefinite $n \times n$ matrix such that $Mu = 0$. Any square matrix whose n row sums are zero has an eigenvalue zero with corresponding eigenvector u. Let W denote the set of all column vectors x that satisfy $x^T x = 1$ and $x^T u = 0$. If M is positive semidefinite, then the second smallest eigenvalue

$$\lambda_{n\ 1}(M) = \min_{x \in W} x^T M x \tag{8.61}$$

which follows from the Rayleigh inequalities in **art.** 152 and the fact that the smallest eigenvalue is $\lambda_n(M) = 0$.

Theorem 41 (Fiedler) *The second smallest eigenvalue $\lambda_{n\ 1}(M)$ of a symmetric, positive definite $n \times n$ matrix M, where $Mu = 0$ obeys*

$$\lambda_{n\ 1}(M) \leq \frac{n}{n-1} \min_{1 \leq j \leq n} m_{jj} \tag{8.62}$$

In addition,

$$2 \max_{1 \leq j \leq n} \sqrt{m_{jj}} \leq \sum_{k=1}^{n} \sqrt{m_{kk}} \tag{8.63}$$

and

$$2 \max_{1 \le j \le n} \sqrt{m_{jj} - \lambda_{n\ 1}(M)\left(1 - \frac{1}{n}\right)} \le \sum_{k=1}^{n} \sqrt{m_{jj} - \lambda_{n\ 1}(M)\left(1 - \frac{1}{n}\right)} \quad (8.64)$$

Proof: Fiedler (1973) observes that the matrix

$$\widetilde{M} = M - \lambda_{n\ 1}(M)\left(I - \frac{1}{n}J\right)$$

is also positive semidefinite. For, let y be any vector in $\mathbb{R}^n$. Then y can be written as $y = c_1 u + c_2 x$ where $x \in W$. Since $\widetilde{M}u = 0$ because $Ju = nu$, it follows with $Jx = u.u^T x = 0$ that

$$y^T \widetilde{M} y = c_2^2 x^T \widetilde{M} x = c_2^2 \left(x^T M x - \lambda_{n\ 1}(M)\right) \ge 0$$

by (8.61). Since any symmetric, positive semidefinite matrix can be considered as a Gram matrix, whose diagonal elements are non negative (see **art. 175**), the minimum diagonal element of $\widetilde{M}$ is non negative,

$$0 \le \min_{1 \le j \le n} \widetilde{m}_{jj} = \min_{1 \le j \le n}\left(m_{jj} - \lambda_{n\ 1}(M)\left(1 - \frac{1}{n}\right)\right)$$

which proves (8.62).

Also M is a Gram matrix, i.e., $M = A^T A$ and $m_{ij} = a_i^T a_j$, where $M = M^T$ is symmetric. The fact that $Mu = 0$ translates to $Au = 0$. This implies that the column vectors $a_1, a_2, \ldots, a_n$ of A obey $\sum_{k=1}^{n} a_k = 0$. Hence, $a_j = -\sum_{k=1, k \ne j}^{n} a_k$, and taking the Euclidean norm of both sides leads to

$$|a_j| \le \sum_{k=1; k \ne j}^{n} |a_k|$$

Since this inequality holds for any $1 \le j \le n$, it also holds for $\max_{1 \le j \le n} |a_j|$,

$$2 \max_{1 \le j \le n} |a_j| \le \sum_{k=1}^{n} |a_k|$$

With $m_{ii} = |a_i|^2$, we arrive at (8.63), which, when applied to $\widetilde{M}$, yields (8.64). □

8.7 Interlacing

178. *The resolvent.* The resolvent of matrix A is defined as $(xI - A)^{-1}$ and is related (**art. 148**) to the adjoint matrix $Q(x) = (xI - A)^{-1} c_A(x)$, where $c_A(x)$ is the characteristic polynomial of A. From the general expression (Meyer, 2000, p. 479) of the inverse of a matrix B,

$$B^{-1} = \frac{\text{adj}B}{\det B}$$

where the adjugate $\text{adj}B$ is the transpose of the matrix of cofactors of B. A cofactor

of element (i, j) is $(-1)^{i+j} \det \widetilde{B}_{ij}$, where $\widetilde{B}_{ij}$ is the matrix obtained from B by deleting the i th row and the j th column. Applied to the diagonal element of $(xI - A)^{-1}$ yields

$$(xI - A)_{jj}^{-1} = \frac{\det \left(xI - A_{\setminus \{j\}}\right)}{\det \left(xI - A\right)} \tag{8.65}$$

where $A_{\setminus \{j\}}$ is the $(n-1) \times (n-1)$ matrix obtained from A by deleting the j th row and column. Furthermore, from the general expression of the derivative of a determinant (Meyer, 2000, p. 471), we find that

$$\frac{d}{dx} \det \left(xI - A\right) = \sum_{j=1}^{n} \det \left(xI - A_{\setminus \{j\}}\right)$$

Hence,

$$\sum_{j=1}^{n} (xI - A)_{jj}^{-1} = \frac{\frac{d}{dx} \det \left(xI - A\right)}{\det \left(xI - A\right)} = \frac{d}{dx} \log \det \left(xI - A\right)$$

Applying (8.32) for a symmetric matrix A to the function $f(y) = \frac{1}{x-y}$, which is everywhere analytic except for $x = y$, yields

$$(xI - A)^{-1} = \sum_{k=1}^{n} \frac{1}{x - \lambda_k} E_k \tag{8.66}$$

After taking the trace of both sides and recalling from **art.** 157 that $\text{trace}(E_k) = m_k$, we finally arrive at

$$\sum_{j=1}^{n} (xI - A)_{jj}^{-1} = \sum_{k=1}^{n} \frac{m_k}{x - \lambda_k} = \frac{d}{dx} \log \det \left(xI - A\right)$$

179. *Christoffel Darboux formula for resolvents.* The resolvent $(xI - A)^{-1}$ of matrix A obeys

$$(xI - A)^{-1} - (yI - A)^{-1} = (y - x)(xI - A)^{-1}(yI - A)^{-1}$$

which is verified by left multiplication by $(yI - A)$ and right multiplication by $(xI - A)$. With $B^{-1} = \frac{\text{adj} B}{\det B}$,

$$\frac{\text{adj}\,(xI - A)}{\det\,(xI - A)} - \frac{\text{adj}\,(yI - A)}{\det\,(yI - A)} = (y - x)\frac{\text{adj}\,(xI - A)}{\det\,(xI - A)}\frac{\text{adj}\,(yI - A)}{\det\,(yI - A)}$$

After multiplying both sides by $(y - x)^{-1} \det\,(xI - A) \det\,(yI - A)$, the element ij of the resulting matrix equation is

$$t_{ij} = \frac{\text{adj}_{ij}\,(xI - A)\det\,(yI - A) - \text{adj}_{ij}\,(yI - A)\det\,(xI - A)}{y - x}$$

$$= \sum_{k=1}^{n} \text{adj}_{ik}\,(xI - A)\,\text{adj}_{kj}\,(yI - A)$$

Since both the adjugate and the determinant of $xI - A$ are polynomials in x of degree $n - 1$ and n, respectively, the Christoffel Darboux identity reflects a polynomial identity, whose strength was first applied in the study of orthogonal polynomials (see **art.** 249). In particular, the limit $y \to x$ results in

$$\lim_{y \to x} t_{ij} = \text{adj}_{ij} (xI - A) \frac{d}{dx} \det (xI - A) - \frac{d}{dx} \text{adj}_{ij} (xI - A) \det (xI - A)$$

$$= \sum_{k=1}^{n} \text{adj}_{ik} (xI - A) \, \text{adj}_{kj} (xI - A)$$

If $i = j$ and A is symmetric (such that $\text{adj} A$ is symmetric), then

$$\text{adj}_{ii} (xI \quad A) \frac{d \det (xI \quad A)}{dx} \quad \frac{d \text{adj}_{ii} (xI \quad A)}{dx} \det (xI \quad A) = \sum_{k \ 1}^{n} (\text{adj}_{ik} (xI \quad A))^2$$

$$(8.67)$$

By using the same arguments as in **art.** 254, the above expression implies that the zeros of the polynomial $p(x) = \text{adj}_{ii} (xI - A)$ and the polynomial $q(x) = \det (xI - A)$ interlace. Here, we follow the proof of Godsil (1993). First, let z be a zero of $p(x)$ with multiplicity m_p and a zero of $q(x)$ with multiplicity m_q. Both of the two terms on the left hand side of (8.67) have a zero at z of multiplicity $m_p + m_q - 1$. The right hand side consists of a sum of squares, such that each term must have a zero at z of multiplicity at least $m_p + m_q - 1$. Now, the $k = i$ th term has a zero at z of multiplicity $2m_p$. Thus, $2m_p \geq m_p + m_q - 1$, implying that $m_p - m_q \geq -1$ and that $\frac{p(x)}{q(x)}$ is a rational function with only simple poles. Further, the residue r_z of $\frac{p(x)}{q(x)}$ at $x \to z$ is

$$r_z = \lim_{x \to z} \frac{p(x)(x - z)}{q(x)} = \lim_{x \to z} \frac{p(x)}{q'(x)} \frac{q'(x)(x - z)}{q(x)} = m_q \lim_{x \to z} \frac{p(x)}{q'(x)}$$

because $q(x) = (x - z)^{m_q} s(x)$ and the polynomial $s(z) \neq 0$. At $x = z$ and, when $q(z) = 0$, (8.67) shows that $p(x) q'(x)$ is positive. A rational function $\frac{p(x)}{q(x)}$ with simple poles that possess a positive residue implies that the zeros of the polynomials $p(x)$ and $q(x)$ interlace. **Art.** 180 presents another proof.

180. *Interlacing.* For any $n \times 1$ vector y, we obtain from (8.66) for a symmetric matrix A that

$$\phi_y (x) = y^T (xI - A)^{-1} y = \sum_{k=1}^{n} \frac{y^T E_k y}{x - \lambda_k}$$

which implies that the rational function $\phi_y (x)$ has simple poles at the real eigen values of A. Differentiation with respect to x yields

$$\frac{d\phi_y (x)}{dx} = - \sum_{k=1}^{n} \frac{y^T E_k y}{(x - \lambda_k)^2}$$

Applying (8.32) to the function $f(y) = \frac{1}{(x-y)^2}$ shows that

$$(xI - A)^{-2} = \sum_{k=1}^{n} \frac{1}{(x - \lambda_k)^2} E_k$$

from which

$$y^T (xI - A)^{-2} y = \sum_{k=1}^{n} \frac{y^T E_k y}{(x - \lambda_k)^2} = -\frac{d\phi_y(x)}{dx}$$

Since

$$y^T (xI - A)^{-2} y = y^T (xI - A)^{-1} (xI - A)^{-1} y$$
$$= y^T \left((xI - A)^{-1}\right)^T (xI - A)^{-1} y = \left\| (xI - A)^{-1} y \right\|_2^2 \geq 0$$

we observe that $\frac{d\phi_y(x)}{dx}$ is always strictly negative whenever x is not a pole of $\phi_y(x)$. This implies that each zero of $\phi_y(x)$ must be simple and lying between two consec utive poles, i.e., eigenvalues of A, of $\phi_y(x)$. As this result holds for any vector y, we find, by choosing $y = e_j$ equal to the base vector e_j, that $\phi_{e_j}(x) = (xI - A)_{jj}^{-1}$. **Art.** 178, in particular (8.65), then indicates that $\det\left(xI - A_{\backslash\{j\}}\right)$ has simple zeros that lie between the zeros of $\det(xI - A)$. Hence, all eigenvalues of the symmetric matrix $A_{\backslash\{j\}}$ lie in between eigenvalues of $A = A^T$,

$$\lambda_{i+1}(A) \leq \lambda_i \left(A_{\backslash\{j\}}\right) \leq \lambda_i(A)$$

for any $1 \leq i \leq n - 1$. This property is called *interlacing*. Since it also applies to a principal submatrix of $A_{\backslash\{j\}}$ obtained by deleting a same row and column, we arrive at the general interlacing theorem:

Theorem 42 (Interlacing) *For a real symmetric matrix $A_{n\times n}$ and any principal submatrix $B_{m\times m}$ of A obtained by deleting $n - m$ same rows and columns in A, the eigenvalues of B interlace with those of A as*

$$\lambda_{n-m+i}(A) \leq \lambda_i(B) \leq \lambda_i(A) \tag{8.68}$$

for any $1 \leq i \leq m$.

Also the zeros of orthogonal polynomials (**art.** 254) are interlaced. There is an interesting corollary of Theorem 42:

Corollary 1 *Let A be a real symmetric $n \times n$ matrix with eigenvalues $\lambda_n(A) \leq \lambda_{n-1}(A) \leq \cdots \leq \lambda_1(A)$ and ordered diagonal elements $d_n \leq d_{n-1} \leq \cdots \leq d_1$ then, for any $1 \leq k \leq n$, it holds that*

$$\sum_{j=1}^{k} d_j \leq \sum_{j=1}^{k} \lambda_j(A)$$

Proof: Let B denote the principal submatrix of A obtained by deleting the rows and columns containing the $n-k$ smallest diagonal elements $d_{k+1}, d_{k+2}, \ldots, d_n$. By (8.7), we have that $\text{trace}(B) = \sum_{j=1}^{k} \lambda_j(B)$ and, by construction of B, $\text{trace}(B) = \sum_{j=1}^{k} d_j$. The Interlacing Theorem provides the inequality (8.68) from which

$$\sum_{j=1}^{k} \lambda_j(B) \leq \sum_{j=1}^{k} \lambda_j(A)$$

Combining the relations proves the corollary. $\qquad\square$

181. *Strict interlacing.* We present yet another derivation of the interlacing prin ciple that allows us to specify strict inequalities when we possess additional infor mation. Let us consider the symmetric $n \times n$ matrix A_n, which we write in terms of the $(n-1) \times (n-1)$ symmetric matrix $A_{n\ 1}$ by adding the last column and row as

$$A_n = \begin{bmatrix} A_{n\ 1} & v_{(n\ 1) \times 1} \\ \left(v^T\right)_{1 \times (n\ 1)} & a_{nn} \end{bmatrix}$$

where the $(n-1) \times 1$ vector $v = (a_{1n}, a_{2n}, \ldots, a_{n\ 1,n})$. The characteristic polyno mial of A_n is, invoking (8.79),

$$\det\left(A_n - \lambda I\right) = \det \begin{bmatrix} A_{n\ 1} - \lambda I & v \\ v^T & a_{nn} - \lambda \end{bmatrix}$$

$$= \det\left(A_{n\ 1} - \lambda I\right) \det\left(a_{nn} - \lambda - \left(v^T \left(A_{n\ 1} - \lambda I\right)^{\ 1} v\right)_{1 \times 1}\right)$$

and

$$\det\left(A_n - \lambda I\right) = \left(a_{nn} - \lambda - v^T \left(A_{n\ 1} - \lambda I\right)^{\ 1} v\right) \det\left(A_{n\ 1} - \lambda I\right) \qquad (8.69)$$

For any symmetric matrix $A_{n\ 1}$, the resolvent can be expressed via (8.66) in **art.** 178 as

$$\left(A_{n\ 1} - \lambda I\right)^{\ 1} = \sum_{m=1}^{n\ 1} \frac{x_m x_m^T}{\xi_m - \lambda}$$

where $x_1, x_2, \ldots, x_{n\ 1}$ are the orthogonal eigenvectors of $A_{n\ 1}$, belonging to the eigenvalues $\xi_1 \geq \xi_2 \geq \ldots \geq \xi_{n\ 1}$, respectively. Hence,

$$v^T \left(A_{n\ 1} - \lambda I\right)^{\ 1} v = \sum_{m=1}^{n\ 1} \frac{\left(v^T x_m\right)^2}{\xi_m - \lambda}$$

and (8.69) is written with the projection[8] $c_m = v^T x_m$ of the vector v on the

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[8] The values $(c_1, c_2, \ldots, c_{n-1})$ can be regarded as the coordinates of the point v in the $n\ 1$ dimensional space with respect to the coordinate axes generated by the orthogonal eigenvectors of A_{n-1}.

eigenvector x_m as

$$\frac{\det (A_n - \lambda I)}{\det (A_{n-1} - \lambda I)} = a_{nn} - \lambda - \sum_{m=1}^{n-1} \frac{c_m^2}{\xi_m - \lambda}$$

Since $\det (A_{n-1} - \lambda I) = \prod_{k=1}^{n-1} (\xi_k - \lambda)$ as shown in **art. 138**, we find the characteristic polynomial of A_n,

$$c_{A_n} (\lambda) = \det (A_n - \lambda I) = (a_{nn} - \lambda) \prod_{k=1}^{n-1} (\xi_k - \lambda) - \sum_{m=1}^{n-1} c_m^2 \prod_{k=1; k \neq m}^{n-1} (\xi_k - \lambda) \quad (8.70)$$

Equation (8.70) shows that

$$c_{A_n} (\xi_q) = (-1)^{n-q} c_q^2 \prod_{k=1}^{q-1} |\xi_k - \xi_q| \prod_{k=q+1}^{n-1} |\xi_k - \xi_q| \quad (8.71)$$

A number of interesting conclusions can be derived from (8.70) and (8.71). First, if $\xi_q = \xi_{q+1}$ is an eigenvalue of A_{n-1} with multiplicity larger than 1, then (8.71) indicates that $c_{A_n} (\xi_q) = 0$, implying that ξ_q is also an eigenvalue of A_n. Eigenvalues of A_{n-1} with multiplicity exceeding 1 are found as a degenerate case of the simple eigenvalue situation when $\xi_q \to \xi_{q+l}$ with $l > 1$. Thus, we assume next that all eigenvalues of A_{n-1} are distinct and simple such that the product of the absolute values of the differences of eigenvalues in (8.71) is strict positive. Then, (8.71) shows that the eigenvalue ξ_q of A_{n-1} cannot be an eigenvalue of A_n, unless $c_q = 0$, which means that v is orthogonal to the eigenvector x_q. If v is not orthogonal to any eigenvector of A_{n-1}, then $c_m \neq 0$ for $1 \leq m \leq n-1$ and $c_{A_n} (\xi_q) \neq 0$ for $1 \leq q \leq n-1$. Moreover, $c_{A_n} (\xi_q)$ is alternatingly negative, starting from $q = n-1$, then positive for $q = n-2$, again negative for $q = n-3$, etc. Since the polynomial $c_{A_n} (x) = (-x)^n + O (x^{n-1})$ for large x as follows from (8.70), there is a zero smaller than ξ_{n-1} (because $c_{A_n} (\xi_{n-1}) < 0$ and $\lim_{x \to -\infty} c_{A_n} (x) > 0$) and a zero larger than ξ_1 (because $(-1)^{n-1} c_{A_n} (\xi_1) > 0$ and $\lim_{x \to \infty} (-1)^{n-1} c_{A_n} (x) < 0$). Since all zeros of $c_{A_n} (x)$ are real (**art. 151**) and the total number of zeros is n (**art. 196**), all zeros of $c_{A_n} (x)$ are simple and there is precisely one zero of $c_{A_n} (x)$ in between two consecutive zeros of $c_{A_{n-1}} (x)$.

This argument presents another derivation of the interlacing principle in **art. 180**. But, the conclusion is more precise and akin to interlacing for orthogonal polynomials (**art. 254**): if the vector v is not orthogonal to any eigenvector of A_{n-1}, which is equivalent to the requirement that $c_m \neq 0$ for $1 \leq m \leq n-1$, then the interlacing is strict in the sense that

$$\lambda_n (A_n) < \lambda_{n-1} (A_{n-1}) < \lambda_{n-1} (A_n) < \ldots < \lambda_1 (A_{n-1}) < \lambda_1 (A_n)$$

Only if v is orthogonal to some eigenvectors, the corresponding eigenvalues are the same for A_n and A_{n-1}.

If v is proportional to an eigenvector, say $v = c_q x_q$, then $c_m = 0$ for all $1 \leq m \leq$

$n-1$, except when $m=q$, such that (8.70) reduces to

$$\det\left(A_n-\lambda I\right)=(a_{nn}-\lambda)\prod_{k=1}^{n\ 1}(\xi_k-\lambda)-c_q^2\prod_{k=1;k\neq q}^{n\ 1}(\xi_k-\lambda)$$

$$=\left\{(a_{nn}-\lambda)(\xi_q-\lambda)-c_q^2\right\}\prod_{k=1;k\neq q}^{n\ 1}(\xi_k-\lambda)$$

which shows that $\det\left(A_n-\lambda I\right)$ and $\det\left(A_{n\ 1}-\lambda I\right)$ have $n-2$ eigenvalues in common and only ξ_q and the zeros of the quadratic equation are different. Indeed, ξ_q is not a zero of $p_2\left(\lambda\right)=(a_{nn}-\lambda)(\xi_q-\lambda)-c_q^2$ because $p_2\left(\xi_q\right)=-c_q^2\neq0$, by construction. This observation is readily extended: if v is a linear combination of l eigenvectors, then there are $n-1-l$ eigenvalues in common. From (8.70) with $c_{l+1}=c_{l+2}=\ldots=c_{n\ 1}=0$, we have

$$\det\left(A_n-\lambda I\right)=(a_{nn}-\lambda)\prod_{k=1}^{n\ 1}(\xi_k-\lambda)-\sum_{m=1}^{l}c_m^2\prod_{k=1;k\neq m}^{l}(\xi_k-\lambda)\prod_{k=l+1}^{n\ 1}(\xi_k-\lambda)$$

$$=p_{l+1}\left(\lambda\right)\prod_{k=l+1}^{n\ 1}(\xi_k-\lambda)$$

where the polynomial is

$$p_{l+1}\left(\lambda\right)=(a_{nn}-\lambda)\prod_{k=1}^{l}(\xi_k-\lambda)-\sum_{m=1}^{l}c_m^2\prod_{k=1;k\neq m}^{l}(\xi_k-\lambda)$$

We see that $p_{l+1}\left(\xi_q\right)=-c_q^2\neq0$, for $1\leq q\leq l$, by construction and that the real $l+1$ zeros of $p_{l+1}\left(\lambda\right)$ determine the zeros of $c_{A_n}\left(x\right)$, that are different from those of $c_{A_{n\ 1}}\left(x\right)$.

In summary, if we build up the matrix A_n by iterating from $n=2$ and requiring in each iteration i that the corresponding $(i-1)\times1$ vector v is not orthogonal to any eigenvector of $A_{i\ 1}$, then each matrix in the sequence $A_2,A_3,\ldots,A_n$ has only simple eigenvalues, that all interlace over $2\leq i\leq n$. Their associated characteristic polynomials are very likely a set of orthogonal polynomials.

In order to have simple, distinct eigenvalues, it is sufficient for A_2 that all ele ments in the upper triangular part including the diagonal are different. However, the statement that "the symmetric matrix A_n has only real, simple eigenvalues provided all its upper triangular (including the diagonal) elements are different" is not correct for $n>2$ as follows from the counter example[9]

$$A_3=\begin{bmatrix}9&3&6\\3&1&2\\6&2&4\end{bmatrix}=A_3^T$$

because the eigenvalues of A_3 are $14,0,0$. In fact, A_3 is the $n=3$ case of a

---

[9] This example is due to F.A. Kuipers.

Fibonacci product matrix A_n, with elements $a_{ij} = F_{i+1}F_{j+1}$, where F_i denotes the i th Fibonacci number. Since $F_{i+1}F_{j+1}$ and $F_{n+1}F_{m+1}$ are only equal if $i = m$ and $j = n$, all elements in the upper triangular part are different. Since all rows are dependent, we have $n - 1$ eigenvalues equal to 0 and one eigenvalue equal to the sum of the diagonal elements, $\sum_{j=1}^{n} F_{j+1}^2$.

Although not correct for $n > 2$, we provide a probabilistic argument that the statement is *in most, but not all cases* correct. A random vector v has almost surely all real elements (components) different. In additional, such a random vector v is almost never orthogonal to any of the $n - 1$ given orthogonal eigenvectors of $A_{n\ 1}$, that span the $n - 1$ dimensional space. Intuitively, one may think of a unit sphere in $n = 3$ dimensions in which the eigenvectors form an orthogonal coordinate axis. The (normalized) vector v is a point on the surface of that unit sphere. The orthogonality requirement translates to three circles on the sphere's surface, each of them passing through two orthogonal eigenvector points. The vector v is not allowed to lie on such a circle. These circles occupy a region with negligible area, thus they have Lesbegue measure zero on that surface. Hence, the probability that v coincides with such a forbidden region is almost zero. Geometric generalizations to higher dimensions are difficult to imagine, but the argument, that the forbidden "orthogonality" regions have a vanishingly small probability to be occupied by a random vector, also holds for $n > 3$. In practice, most matrices A_n that obey the statement have distinct eigenvalues.

182. *General interlacing.* **Art.** 180, in particular Theorem 42, has been generalized by Haemers (1995):

Theorem 43 (Generalized Interlacing) *Let A be a real symmetric $n \times n$ matrix and S be a real $n \times m$ orthogonal matrix satisfying $S^T S = I$. Denote the eigenvector v_k belonging to the eigenvalue $\lambda_k(B)$ of the $m \times m$ matrix $B = S^T A S$. Then,*

  (i) *the eigenvalues of B interlace with those of A;*
 (ii) *if $\lambda_k(B) = \lambda_k(A)$ (or $\lambda_k(B) = \lambda_{n\ m+k}(A)$) for some $k \in [1, m]$, then Sv_k is an eigenvector of A belonging to $\lambda_k(A)$;*
(iii) *if there exists an integer $k \in [0, m]$ such that $\lambda_j(B) = \lambda_j(A)$ for $1 \leq j \leq k$ and $\lambda_j(B) = \lambda_{n\ m+j}(A)$ for $k + 1 \leq j \leq m$, then $SB = AS$.*

Proof: The Rayleigh's inequalities (8.27) in **art.** 152, applied to an $m \times 1$ vector s_j be a vector belonging to the space spanned by the eigenvectors $\{v_1, v_2, \ldots, v_j\}$, are

$$\frac{s_j^T B s_j}{s_j^T s_j} \geq \lambda_j(B)$$

Since

$$\frac{s_j^T B s_j}{s_j^T s_j} = \frac{(Ss_j)^T A S s_j}{(Ss_j)^T S s_j}$$

Rayleigh's principle, now applied to the vector Ss_j, states that the right hand side is smaller than $\lambda_j(A)$ provided Ss_j belongs to the space spanned by $\{x_j, x_j, \ldots, x_n\}$, the last $n + 1 - j$ eigenvectors of A. In that case, Ss_j can be written as a linear combination,

$$Ss_j = \sum_{k=j}^{n} c_k x_k$$

Using the orthogonality $S^{-1} = S^T$,

$$s_j = \sum_{k=j}^{n} c_k S^T x_k$$

Hence, if we choose s_j belonging to the space spanned by $\{v_1, v_2, \ldots, v_j\}$ and orthogonal to the space spanned by $\{S^T x_1, S^T x_2, \ldots, S^T x_{j-1}\}$, then $\lambda_{j+1}(A) \leq \lambda_j(B) \leq \lambda_j(A)$ for any $1 \leq j \leq m$. If the same reasoning is applied to $-A$ and $-B$, we obtain $\lambda_j(B) \geq \lambda_{n-m+j}(A)$, thereby proving (i). Equality, occurring in the Rayleigh inequalities, $\lambda_j(B) = \lambda_j(A)$, means that the $s_j = v_j$ is an eigenvector of B belonging to the eigenvalue $\lambda_j(B)$ *and* that $Ss_j = Sv_j = x_j$ is an eigenvector of A belonging to the eigenvalue $\lambda_j(A)$. This proves (ii). The last point (iii) implies, using (ii), that $Sv_1, Sv_2, \ldots, Sv_m$ is an orthonormal set of eigenvectors of A belonging to the eigenvalues $\lambda_1(B), \lambda_2(B), \ldots, \lambda_m(B)$. Left multiplying the eigenvalue equation $Bv_j = \lambda_j(B)v_j$ by S yields

$$SBv_j = \lambda_j(B)Sv_j = \lambda_j(A)x_j = Ax_j = ASv_j$$

from which $SB = AS$ follows because all $1 \leq j \leq m$ eigenvector span the m dimensional space.   □

By choosing $S = \begin{bmatrix} I_{m \times m} & O_{m \times (n-m)} \end{bmatrix}^T$, we find that B is just a principal submatrix of A. This observation shows that Theorem 42 is a special case of the general Theorem 43, which was already known to Cauchy.

183. *Interlacing and the sum $A + B$.*

Lemma 8 *For symmetric $n \times n$ matrices A, B, it holds that*

$$\lambda_n(B) + \lambda_k(A) \leq \lambda_k(A + B) \leq \lambda_k(A) + \lambda_1(B) \qquad (8.72)$$

Proof: The proof is based on the Rayleigh's inequalities (**art.** 152) of eigenvalues (see, e.g., Wilkinson (1965, pp. 101 102)).   □

An extension of Lemma 8 is, for $k + j - 1 \leq n$,

$$\lambda_{k+j-1}(A + B) \leq \lambda_k(A) + \lambda_j(B)$$

which is also called an *interlacing* property. These inequalities are also known as the Courant Weyl inequalities and also hold for Hermitian matrices.

Lemma 9 *If*

$$X = \begin{bmatrix} A & C \\ C^T & B \end{bmatrix}$$

is a real symmetric matrix, where A and B are square, and consequently symmetric, matrices, then

$$\lambda_{\max}(X) + \lambda_{\min}(X) \leq \lambda_{\max}(A) + \lambda_{\max}(B) \tag{8.73}$$

Proof: See, e.g., Biggs (1996, p. 56). $\qquad\square$

Theorem 44 (Wielandt-Hoffman) *For symmetric matrices A and B, it holds that*

$$\sum_{k=1}^{n} (\lambda_k(A+B) - \lambda_k(A))^2 \leq \sum_{k=1}^{n} \lambda_k^2(B) \tag{8.74}$$

Proof: See, e.g., Wilkinson (1965, pp. 104 108). $\qquad\square$

We can rewrite (8.74) with $C = A + B$ and $B = C - A$ as

$$\sum_{k=1}^{n} \lambda_k^2(A) + \sum_{k=1}^{n} \lambda_k^2(C) - \sum_{k=1}^{n} \lambda_k^2(C-A) \leq 2\sum_{k=1}^{n} \lambda_k(A)\lambda_k(C)$$

Using (8.20), we have

$$2\sum_{k=1}^{n} \lambda_k(A)\lambda_k(C) \geq \operatorname{trace}(A^2) + \operatorname{trace}(C^2) - \operatorname{trace}\left((C-A)^2\right)$$

$$= \operatorname{trace}\left(A^2 + C^2 - (C-A)^2\right)$$

$$= \operatorname{trace}(CA + AC) = 2\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}c_{ij}$$

Hence, an equivalent form of the Wielandt Hoffman Theorem 44 for symmetric matrices A and B is

$$\operatorname{trace}(AB) \leq \sum_{k=1}^{n} \lambda_k(A)\lambda_k(B) \tag{8.75}$$

8.8 Eigenstructure of the product AB

184. *Eigenvalues of the product AB.*

Lemma 10 *For all matrices $A_{n\times m}$ and $B_{m\times n}$ with $n \geq m$, it holds that $\lambda(AB) = \lambda(BA)$ and $\lambda(AB)$ has $n - m$ extra zero eigenvalues.*

Proof: Consider the matrix identities

$$\begin{bmatrix} I_{n\times n} & O_{n\times m} \\ -B_{m\times n} & \mu I_{m\times m} \end{bmatrix} \begin{bmatrix} \mu I_{n\times n} & A_{n\times m} \\ B_{m\times n} & \mu I_{m\times m} \end{bmatrix} = \begin{bmatrix} \mu I_{n\times n} & A_{n\times m} \\ O_{m\times n} & \left(\mu^2 I - BA\right)_{m\times m} \end{bmatrix}$$

and

$$\begin{bmatrix} \mu I_{n\times n} & -A_{n\times m} \\ O_{m\times n} & I_{m\times m} \end{bmatrix} \begin{bmatrix} \mu I_{n\times n} & A_{n\times m} \\ B_{m\times n} & \mu I_{m\times m} \end{bmatrix} = \begin{bmatrix} \left(\mu^2 I - AB\right)_{n\times n} & O_{n\times m} \\ B_{m\times n} & \mu I_{m\times m} \end{bmatrix}$$

Taking the determinants of both sides of each identity and denoting

$$X = \begin{bmatrix} \mu I_{n\times n} & A_{n\times m} \\ B_{m\times n} & \mu I_{m\times m} \end{bmatrix}$$

gives respectively

$$\mu^m \det X = \mu^n \det\left(\mu^2 I - BA\right)$$
$$\mu^n \det X = \mu^m \det\left(\mu^2 I - AB\right)$$

from which it follows, with $\lambda = \mu^2$, that $\lambda^{n-m} \det\left(BA - \lambda I\right) = \det\left(AB - \lambda I\right)$, which is an equation of two polynomials in λ. Equating corresponding powers in λ proves Lemma 10. $\square$

Lemma 11 *If square matrices $A_{n\times n}$ and $B_{n\times n}$ commute such that $AB = BA$, then the set of eigenvectors of A is the same as the set of eigenvectors of B provided that all n eigenvectors are independent. The converse more generally holds: if any two matrices A and B have a common complete set of eigenvectors, then $AB = BA$.*

Proof: If x_k is an eigenvector of A corresponding to eigenvalue λ_k, then $Ax_k = \lambda_k x_k$. Left multiplying both sides by B and using the commutative property yields $A\left(Bx_k\right) = \lambda_k\left(Bx_k\right)$, which implies that, to any eigenvector x_k with eigen value λ_k, the matrix A also possesses an eigenvector Bx_k with same eigenvalue λ_k. Since eigenvectors are linearly independent and since the set of n eigenvectors $\{x_1, x_2, \ldots, x_n\}$ spans the n dimensional space, the eigenvector $Bx_k = \mu_k x_k$, which means that x_k is also an eigenvector of B.

The converse follows from **art.** 142 since $A = X\text{diag}(\lambda_k)X^{-1}$ and, similarly, $B = X\text{diag}(\mu_k)X^{-1}$. Indeed,

$$AB = X\text{diag}\left(\lambda_k\right)X^{-1}X\text{diag}\left(\mu_k\right)X^{-1} = X\text{diag}\left(\lambda_k\mu_k\right)X^{-1}$$
$$BA = X\text{diag}\left(\mu_k\right)X^{-1}X\text{diag}\left(\lambda_k\right)X^{-1} = X\text{diag}\left(\lambda_k\mu_k\right)X^{-1}$$

shows that $AB = BA$. $\square$

If all eigenvalues are distinct, all eigenvectors are independent. However, in case of multiple eigenvalues, the situation can be more complex such that there are fewer than n independent eigenvectors. In that case, the Lemma 11 is not applicable. A direct consequence of Lemma 11 is that, for commuting matrices A and B, the eigenvalues of $A + B$ are $\lambda_k + \mu_k$ and both eigenvalues belong to the

same eigenvector x_k. If matrices are not commuting, remarkably little can be said about the eigenvalues of $A + B$, given the spectra of A and B (see also **art.** 154).

185. *Kronecker product.* The Kronecker product of the $n \times m$ matrix A and the $p \times q$ matrix B is the $np \times mq$ matrix $A \otimes B$, where

$$
A \otimes B = \begin{bmatrix}
a_{11}B & a_{12}B & \cdots & a_{1m}B \\
a_{21}B & a_{22}B & \cdots & a_{2m}B \\
\vdots & \vdots & \ddots & \vdots \\
a_{n1}B & a_{n2}B & \cdots & a_{nm}B
\end{bmatrix}
$$

The Kronecker product $A \otimes B$ features many properties (Meyer, 2000, p. 597). The eigenvalues of $A_{n \times n} \otimes B_{m \times m}$ are the nm numbers $\{\lambda_j (A) \lambda_k (B)\}_{1 \le j \le n, 1 \le k \le m}$. Likewise, the set of eigenvalues of $I_m \otimes A_{n \times n} + B_{m \times m} \otimes I_n$ equals the set of nm eigenvalues $\{\lambda_j (A) + \lambda_k (B)\}_{1 \le j \le n, 1 \le k \le m}$.

186. *The commutator of a matrix.* Consider the matrix equation

$$
A_{n \times n} X_{n \times m} + X_{n \times m} B_{m \times m} = C_{n \times m}
$$

that includes the commutator equation, $AX - XA = O$, where X are all matrices that commute with A, as a special case, as well as the Lyapunov equation (Horn and Johnson, 1991, Chapter 4). The matrix equation is written in Kronecker form as

$$
\left(I_m \otimes A_{n \times n} + B_{m \times m}^T \otimes I_n\right) vec\left(X\right) = vec\left(C\right) \tag{8.76}
$$

where the $nm \times 1$ vector is

$$
\begin{aligned}
vec\left(X\right) &= \left(x_1^T, x_2^T, \ldots, x_m^T\right) \\
&= \left(x_{11}, \ldots, x_{n1}, x_{12}, \ldots, x_{n2}, \ldots, x_{1m}, \ldots, x_{nm}\right)
\end{aligned}
$$

where x_j is the j th $n \times 1$ column vector of X. The mixed product property (Meyer, 2000, p. 597),

$$
\left(A_1 \otimes B_1\right)\left(A_2 \otimes B_2\right) = \left(A_1 A_2 \otimes B_1 B_2\right)
$$

shows that

$$
\left(I_m \otimes A_{n \times n}\right)\left(B_{m \times m} \otimes I_n\right) = \left(B_{m \times m} \otimes A_{n \times n}\right) = \left(B_{m \times m} \otimes I_n\right)\left(I_m \otimes A_{n \times n}\right)
$$

In other words, the square $mn \times mn$ matrices $I_m \otimes A_{n \times n}$ and $B_{m \times m} \otimes I_n$ commute. Horn and Johnson (1991) prove that, if w_k is an $n \times 1$ eigenvector of A belonging to $\lambda_k (A)$ and y_l an $m \times 1$ eigenvector of B belonging to $\lambda_l (B)$, then $y_l \otimes w_k$ is an $nm \times 1$ eigenvector of $I_m \otimes A_{n \times n} + B_{m \times m} \otimes I_n$ belonging to the eigenvalue $\lambda_k (A) + \lambda_l (B)$.

The linear equation (8.76) has a unique solution provided none of the eigenvalues $\lambda_k (A) + \lambda_l (B) = 0$ for all $1 \le k \le n$ and $1 \le l \le m$, because $\lambda_l \left(B^T\right) = \lambda_l (B)$ on **art.** 140. Likewise, if $C = O$ in (8.76), the equation $AX - BX = O$ has only a solution, provided $\{\lambda_k (A)\}_{1 \le k \le n} \cap \{\lambda_l (B)\}_{1 \le k \le n} \ne \varnothing$. Thus, when $B = A$,

in which case X is the commutator of A, there are at least n zero eigenvalues of $I_n \otimes A_{n \times n} - A_{n \times n} \otimes I_n$ (and more than n if A has zero eigenvalues) illustrating that there many possible commutators of a matrix A. If $C \neq O$ and $B = -A$ in (8.76), there is no solution for X. A theorem of Shoda, proved in Horn and Johnson (1991, p. 288), states that C can be written as $C = XY - YX$ for some matrices X and Y provided $\text{trace}(C) = 0$.

8.9 Formulae of determinants

The theory of determinants is discussed in historical order up to 1920 by Muir (1930) in five impressive volumes. Muir claims to be comprehensive. His treatise summarizes each paper and relates that paper to others. A remarkably large amount of papers are by his hand. Many papers deal with specially structured determinants that sometimes possess a nice, closed form[10].

187. A determinant of an $n \times n$ matrix A is defined by

$$\det A = \sum_p (-1)^{\sigma(p)} \prod_{j=1}^{n} a_{jk_j} \tag{8.77}$$

where the sum is over all the $n!$ permutations $p = (k_1, k_2, \ldots, k_n)$ of $(1, 2, \ldots, n)$ and $\sigma(p)$ is the number of interchanges between p and the natural order $(1, 2, \ldots, n)$. For example, $p = (1, 3, 2, 4)$ has 1 interchange, $\sigma(p) = 1$, while $p = (4, 3, 2, 1)$ has $\sigma(p) = 2$. Thus, $\sigma(p)$ is the number of interchanges to bring p back to the natural order. The determinant of a non square matrix is not defined.

188. From the Schur identity

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I & O \\ CA^{-1} & I \end{bmatrix} \begin{bmatrix} A & B \\ O & D - CA^{-1}B \end{bmatrix} \tag{8.78}$$

we find that

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det A \det (D - CA^{-1}B) \tag{8.79}$$

and $D - CA^{-1}B$ is called the Schur complement of A. Similarly (see, e.g., Meyer (2000)),

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det D \det (A - BD^{-1}C) \tag{8.80}$$

---

[10] We mention as an example the following $n \times n$ determinant of Scott (1880) in Muir (1930, vol. IV, p. 124), which involves all players of the harmonic, geometric and arithmetic mean inequality (5.15),

$$\begin{vmatrix} 0 & a_1 + a_2 & a_1 + a_3 \\ a_1 + a_2 & 0 & a_2 + a_3 & \cdots \\ a_1 + a_3 & a_2 + a_3 & \ddots \\ \vdots & \vdots & & \ddots \end{vmatrix} \quad \frac{(-2)^{n-1}}{2} \prod_{j=1}^{n} a_j \left\{ \left(\sum_{j=1}^{n} a_j \right) \left(\sum_{j=1}^{n} \frac{1}{a_j} \right) - (n-2)^2 \right\}$$

189. An interesting application of **art.** 188 is

$$\det \begin{bmatrix} A_{n\times n} & -C_{n\times k} \\ D_{k\times n}^T & I_k \end{bmatrix} = \det \left(A_{n\times n} + C_{n\times k} D_{k\times n}^T \right) = \det A \det \left(I_k + D^T A^{-1} C \right)$$
(8.81)

which follows by applying both (8.80) and (8.79). For $k = 1$ and $A = I$ in (8.81), we obtain the "rank one update" formula

$$\det \left(I + cd^T \right) = 1 + d^T c$$
(8.82)

This example shows that interesting relations can be obtained when the inverse of either A or D or both in (8.79) and (8.80) are explicitly known.

190. *Cramer's rule.* The linear set of equations, $Ax = b$, has a unique solution $x = A^{-1}b$ provided $\det A \neq 0$. If we write the matrix A in terms of its column vectors $a_k = (a_{1k}, a_{2k}, \ldots, a_{2k})$, then

$$A = \begin{bmatrix} a_1 & \cdots & a_{k-1} & a_k & a_{k+1} & \cdots & a_n \end{bmatrix}$$

Cramer's rule expresses the unique solution of $x = (x_1, x_2, \ldots, x_n)$ per component as

$$x_k = \frac{\det \begin{bmatrix} a_1 & \cdots & a_{k-1} & b & a_{k+1} & \cdots & a_n \end{bmatrix}}{\det A}$$
(8.83)

Indeed, we can write the matrix A with the k th column replaced by the vector b as

$$A_k = A + (b - a_k) e_k^T$$

where e_k is the k th basis vector. Thus, $y e_k^T$ equals the zero matrix with the k th column replaced by the vector y and it has rank 1. Then,

$$\det A_k = \det \left(A + (b - a_k) e_k^T \right) = \det A \det \left(I + A^{-1} (b - a_k) e_k^T \right)$$

Application of the "rank one update" formula (8.82), recalling that $Ae_k = a_k$ and $e_k = A^{-1} a_k$, yields

$$\det \left(I + A^{-1} (b - a_k) e_k^T \right) = 1 + e_k^T A^{-1} (b - a_k)$$
$$= 1 + e_k^T \left(A^{-1}b - A^{-1}a_k \right)$$
$$= 1 + e_k^T (x - e_k) = x_k$$

which demonstrates (8.83).

191. *Expansion of the determinant of a product.*

Theorem 45 (Binet-Cauchy) *Let $C = AB$ where $A_{m\times n}$ and $B_{n\times m}$. Then,*

$$\det C = \sum_{1 \leq k_1 < k_2 < \cdots < k_m \leq n} \begin{vmatrix} a_{1k_1} & \cdots & a_{1k_m} \\ \vdots & \cdots & \vdots \\ a_{mk_1} & \cdots & a_{mk_m} \end{vmatrix} \begin{vmatrix} b_{k_11} & \cdots & b_{k_m1} \\ \vdots & \cdots & \vdots \\ b_{k_1m} & \cdots & b_{k_mm} \end{vmatrix}$$
(8.84)

Proof: See, e.g., Gantmacher (1959a, pp. 9 10). □

If $B_{n \times m} = (A_{m \times n})^T$ (thus $b_{ij} = a_{ji}$), then the Binet Cauchy formula (8.84) reduces to

$$\det AA^T = \sum_{k_1=1}^{n} \sum_{k_2=k_1+1}^{n} \cdots \sum_{k_m=k_m\ 1+1}^{n} \begin{vmatrix} a_{1k_1} & \cdots & a_{1k_m} \\ \vdots & \cdots & \vdots \\ a_{mk_1} & \cdots & a_{mk_m} \end{vmatrix}^2 \tag{8.85}$$

192. *The Cauchy identity.* The Cauchy identity

$$\sum_{j=1}^{n} x_j^2 \sum_{j=1}^{n} y_j^2 - \left(\sum_{j=1}^{n} x_j y_j \right)^2 = \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} (x_j y_k - x_k y_j)^2 \tag{8.86}$$

is the special case for the dimension $m = 2$ in the Binet Cauchy Theorem 45. Specifically, (8.85) reduces to (8.86) for the matrix $A_{2 \times n} = \begin{bmatrix} x^T \\ y^T \end{bmatrix}$, where x and y are $n \times 1$ vectors. Since the right hand side in the Cauchy identity (8.86) is non negative for real vectors x and y, the Cauchy Schwarz inequality (8.41) written as

$$\sum_{j=1}^{n} x_j^2 \sum_{j=1}^{n} y_j^2 \geq \left(\sum_{j=1}^{n} x_j y_j \right)^2$$

is a consequence of (8.86).

Since $\text{Var}[X] = E[X^2] - (E[X])^2$, Cauchy's equality (8.86) shows that for any random variable X in a specific graph, the variance equals

$$\text{Var}[X] = \frac{1}{n} \sum_{j=1}^{n} x_j^2 - \left(\frac{1}{n} \sum_{j=1}^{n} x_j \right)^2 = \sum_{j=2}^{n} \sum_{k=1}^{j\ 1} \left(\frac{x_j - x_k}{n} \right)^2 \tag{8.87}$$

where the last term sums the square of the difference in realizations of X over all pairs of nodes in the graph.

193. We give an identity for any matrix B due to Jacobi,

$$e^{\text{trace}(B)} = \det e^B \tag{8.88}$$

We present two proofs. The first proof is the general proof. The logarithm $\log(I - C)$ has a formal Taylor series provided all eigenvalues $|\lambda(C)| < 1$,

$$\log(I - C) = \sum_{k=1}^{\infty} \frac{C^k}{k} = \sum_{k=1}^{\infty} C^k \int_0^1 y^{k\ 1} dy = \int_0^1 \sum_{k=0}^{\infty} C^{k+1} y^k dy$$

$$= \int_0^1 C(I - Cy)^{\ 1} dy$$

The relation with the determinant follows from the general definition of the inverse of a matrix, which is $(I - Cy)^{-1} = \frac{1}{\det(I - Cy)} \text{adj}(I - Cy)$. Hence,

$$\log (I - C) = \int_0^1 C \text{adj} (I - Cy) \frac{dy}{\det (I - Cy)}$$

By matrix multiplications and denoting the dimension of the matrix B (and C) by N, we have that

$$\{C \text{adj} (I - Cy)\}_{ij} = \sum_{n=1}^N c_{in} \times \text{cofactor}_{jn} (I - Cy)$$

and

$$\text{trace} \{C \text{adj} (I - Cy)\} = \sum_{j=1}^N \sum_{n=1}^N c_{jn} \times \text{cofactor}_{jn} (I - Cy)$$

Any determinant can be expanded in a sum of cofactors as

$$\det (A) = \sum_{n=1}^N a_{jn} \times \text{cofactor}_{jn} A$$

and the derivative with respect to y is (Meyer, 2000, ex. 6.2.25)

$$\frac{d}{dy} \det (A) = \sum_{j=1}^N \sum_{n=1}^N \frac{da_{jn}}{dy} \times \text{cofactor}_{jn} A$$

$$= \text{trace} \left(\text{adj} A \times \frac{dA}{dy} \right)$$

If $A^{-1} = \frac{\text{adj} A}{\det A}$ exists, then Jacobi's analysis shows that

$$\frac{d}{dy} \det (A) = \det A \text{trace} \left(A^{-1} \times \frac{dA}{dy} \right)$$

Thus,

$$\text{trace} \{C \text{adj} (I - Cy)\} = -\frac{d}{dy} \det (I - Cy)$$

and

$$\text{trace} \log (I - C) = \int_0^1 \text{trace} \{C \text{adj} (I - Cy)\} \frac{dy}{\det (I - Cy)}$$

$$= \int_0^1 \frac{-\frac{d}{dy} \det (I - Cy) \, dy}{\det (I - Cy)} = \log \det (I - Cy)|_0^1$$

$$= \log \det (I - C)$$

We arrive at

$$\text{trace} \log (I - C) = \log \det (I - C) \tag{8.89}$$

By substitution of $B = \log (I - C)$, we find Jacobi's expression (8.88). Finally, the condition that $|\lambda (C)| < 1$ does not restrict the eigenvalues of B.

The second proof is much shorter, but it assumes that all eigenvalues are distinct such that, from the eigenvalue representation, we have $e^B = X \mathrm{diag}(e^{\lambda(B)}) X^{-1}$. Taking the determinant of both sides gives

$$\det e^B = \det X \det \left(\mathrm{diag} \left(e^{\lambda(B)} \right) \right) \det X^{-1} = \prod_{j=1}^{N} e^{\lambda_j(B)}$$

$$= e^{\sum_{j=1}^{N} \lambda_j(B)} = e^{\mathrm{trace} B}$$

After taking the logarithm in (8.88), the trace is expressed in terms of the determinant,

$$\mathrm{trace} (A) = \log \det e^A$$

while by substituting $A = e^B$ in (8.88), Jacobi's identity expresses a determinant as a function of the trace

$$\det A = e^{\mathrm{trace}(\log A)}$$

Expanding the last expression (via Taylor series) shows the relation with the Newton identities (9.3) as demonstrated in **art. 36**.

194. The $n \times n$ Vandermonde matrix of the vector x is defined as[11]

$$V_n (x) = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & x_2^3 & \cdots & x_2^{n-1} \\ 1 & x_3 & x_3^2 & x_3^3 & \cdots & x_3^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^{n-1} \end{bmatrix} \tag{8.90}$$

The Vandermonde matrix appeared earlier in **art. 143** as the eigenvector matrix of the companion matrix.

The Vandermonde determinant obeys the recursion

$$\det V_n (x) = \prod_{j=1}^{n-1} (x_n - x_j) \det V_{(n-1)} (x) \tag{8.91}$$

with $\det V_2 (x) = x_2 - x_1$. Indeed, subtracting the last row from all previous rows

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[11] There are different ways to define the Vandermonde matrix, for instance, by organizing the powers of the vector x in rows (as in **art. 143**) instead of in columns, and by choosing the sequence of powers in either decreasing or increasing order.

and using the algebraic formula $x^k - y^k = (x - y)\sum_{j=0}^{k-1} x^{k-1-j} y^j$ yields

$$\det V_n(x) = \begin{vmatrix} 0 & x_1 - x_n & (x_1 - x_n)(x_1 + x_n) & \cdots & \cdots & x_1^{n-1} - x_n^{n-1} \\ 0 & x_2 - x_n & (x_2 - x_n)(x_2 + x_n) & \cdots & \cdots & x_2^{n-1} - x_n^{n-1} \\ 0 & x_3 - x_n & (x_3 - x_n)(x_3 + x_n) & \cdots & \cdots & x_3^{n-1} - x_n^{n-1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & x_{n-1} - x_n & (x_{n-1} - x_n)(x_{n-1} + x_n) & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^{n-1} \end{vmatrix}$$

After expanding the determinant as $(-1)^n$ times the cofactor of the last element of the first column, the resulting determinant is, after dividing each row r by the factor $x_r - x_n$,

$$\det W_{n-1} = \begin{vmatrix} 1 & x_1 + x_n & x_1^2 + x_1 x_n + x_n^2 & \cdots & \cdots & \sum_{j=0}^{n-2} x_n^{n-2-j} x_1^j \\ 1 & x_2 + x_n & x_2^2 + x_2 x_n + x_n^2 & \cdots & \cdots & \sum_{j=0}^{n-2} x_n^{n-2-j} x_2^j \\ 1 & x_3 + x_n & x_2^2 + x_2 x_n + x_n^2 & \cdots & \cdots & \sum_{j=0}^{n-2} x_n^{n-2-j} x_3^j \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 1 & x_{n-2} + x_n & x_{n-2}^2 + x_{n-2} x_n + x_n^2 & \cdots & \vdots & \vdots \\ 1 & x_{n-1} + x_n & x_{n-1}^2 + x_{n-1} x_n + x_n^2 & \cdots & \cdots & \sum_{j=0}^{n-2} x_n^{n-2-j} x_{n-1}^j \end{vmatrix}$$

A determinant remains unchanged by adding a column multiplied by some number α to another column. Since $\sum_{j=0}^{k-1} x^{k-1-j} y^j = x^{k-1} + y\sum_{j=0}^{k-2} x^{k-2-j} y^j$, we can subsequently multiply each but the last column k by x_n and subtract the result from the column $k+1$ to arrive at $W_{n-1} = V_{n-1}(x)$. This establishes the recursion (8.91). Iterating the recursion (8.91) results in

$$\det V_n(x) = \prod_{1 \le i < j \le n} (x_j - x_i) = \prod_{i=1}^{n} \prod_{j=i+1}^{n} (x_j - x_i) \tag{8.92}$$

195. *Hadamard's inequality.* Consider the matrix $A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$, with as columns the vectors $\{a_k\}_{1 \le k \le n}$. The Hadamard inequality for the determinant, proved in Meyer (2000, p. 469), is

$$|\det A| \le \prod_{k=1}^{n} \|a_k\|_2 = \prod_{k=1}^{n} \sqrt{\sum_{j=1}^{n} |a_{kj}|^2} \tag{8.93}$$

with equality only if all the vectors $a_1, a_2, \ldots, a_n$ are mutually orthogonal, i.e., if $(a_k)^T a_j = \delta_{kj}$ or, when complex $(a_k)^H a_j = \delta_{kj}$, for all pairs (k, j). As proved by Meyer (2000, p. 469), the volume V_n of an n dimensional parallelepiped, a possibly *skewed* rectangular box generated by n independent vectors $a_1, a_2, \ldots, a_n$, equals $V_n = |\det A|$. This relation provides a geometrical interpretation of the determinant. Hadamard's inequality (8.93) asserts that the volume of an n dimensional paral lelepiped generated by the columns of A cannot exceed the volume of a rectangular

box whose sides have length $\|a_k\|_2$. In general, an n dimensional parallelepiped is skewed, i.e., its n independent, generating vectors $a_1, a_2, \ldots, a_n$ are not orthogonal, which geometrically explains Hadamard's inequality (8.93).

We apply the Hadamard inequality (8.93) to the Vandermonde determinant in **art.** 194, where the components of the vector x are ordered as $|x_1| > |x_2| > \ldots > |x_m| > 1 \geq |x_{m+1}| > \ldots > |x_n|$. After dividing the first m rows, corresponding to the components with absolute value larger than 1, by x_j^{n-1} for $1 \leq j \leq m$, we obtain

$$\det V_n(x) = \prod_{j=1}^{m} x_j^{n-1} \begin{vmatrix} x_1^{(n-1)} & x_1^{(n-2)} & x_1^{(n-3)} & x_1^{(n-4)} & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_m^{(n-1)} & x_m^{(n-2)} & x_m^{(n-3)} & x_m^{(n-4)} & \cdots & 1 \\ 1 & x_{m+1} & x_{m+1}^2 & x_{m+1}^3 & \cdots & x_{m+1}^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^{n-1} \end{vmatrix}$$

Since none of the elements in this determinant exceeds in absolute value unity, Hadamard's inequality (8.93) shows that

$$|\det V_n(x)| \leq n^{\frac{n}{2}} \prod_{j=1}^{m} |x_j|^{n-j}$$

with equality if and only if the row vectors are orthogonal. **Art.** 143 shows that orthogonality is only possible if all $x_j = e^{2\pi i \frac{j}{n}}$ corresponding to the zeros of $p_n(z) = a_n(z^n \pm 1)$. Using (8.92) and $|x_j| = 1$ yields

$$\prod_{k=1}^{n} \prod_{j=k+1}^{n} \left| e^{\frac{2\pi i j}{n}} - e^{\frac{2\pi i k}{n}} \right| = n^{\frac{n}{2}} \tag{8.94}$$

9

Polynomials with real coefficients

The characteristic polynomial of real matrices possesses real coefficients. This chapter aims to summarize general results on the location and determination of the zeros of polynomials with mainly real coefficients. The operations here are assumed to be performed over the set $\mathbb{C}$ of complex numbers. Restricting operations to other subfields of $\mathbb{C}$, such as the set $\mathbb{Z}$ of integers or finite fields, is omitted because, in that case, we need to enter an entirely different and more complex area, which requires Galois theory, advanced group theory and number theory. A general outline for the latter is found in Govers *et al.* (2008) and a nice introduction to Galois theory is written by Stewart (2004).

The study of polynomials belongs to one of the oldest researches in mathematics. The insolubility of the quintic, famously proved by Abel and extended by Galois (see **art.** 196 and Govers *et al.* (2008) for more details and for the historical context), shifted the root finding problem in polynomials from pure to numerical analysis. Numerical methods as well as matrix method based on the companion matrix (**art.** 143) are extensively treated by McNamee (2007), but omitted here. A complex function theoretic approach, covering more recent results such as self inversive polynomials and extensions of Grace's Theorem (**art.** 227), is presented by Sheil Small (2002) and by Milovanović *et al.* (1994), who also list many polynomial inequalities. In addition, Milovanović *et al.* (1994) treat polynomial extremal problems of the type: given that the absolute value of a polynomial is bounded in some region of the complex plane, how large can its derivative be in that region?

9.1 General properties

196. A fundamental theorem of algebra, first proved by Gauss and later by Liouville (Titchmarsh, 1964, p. 118), states that any polynomial of degree n has precisely n zeros in the complex plane. If these zeros coincide, we count zeros according to their multiplicity. Thus, if there are $l < n$ zeros and a zero z_k has multiplicity m_k, then the fundamental theorem states that $\sum_{k=1}^{l} m_k = n$. In the sequel, we

represent zeros as if they are single, however, with the convention that a coinciding zero z_k with multiplicity m_k is counted m_k times.

Let $p_n(z)$ denote a polynomial of degree n defined by

$$p_n(z) = \sum_{k=0}^{n} a_k z^k = a_n \prod_{k=1}^{n} (z - z_k) \tag{9.1}$$

where $\{z_k\}_{1 \leq k \leq n}$ is the set of n zeros and the coefficient a_k (for $0 \leq k \leq n$) is a (finite) complex number. Moreover, we require that $a_n \neq 0$, otherwise the polynomial is not of degree n. If $a_n = 1$, which is an often used normalization, the polynomial is called "monic".

Once the set of zeros is known, the coefficients a_k can be computed by multiplying out the product in (9.1). The other direction, the determination of the set of zeros given the set coefficients $\{a_k\}_{0 \leq k \leq n}$, proves to be much more challenging. Abel and Galois have shown that only up to degree $n = 4$ explicit relations of the zeros exist in terms of a finite number of elementary operations such as additions, subtractions, multiplications, divisions and radicals on the coefficients. The solution of the cubic ($n = 3$) and quartic ($n = 4$) can be found, for example, in Stewart (2004) and Milovanović *et al.* (1994). An important aspect of the theory of polynomials thus lies in the determination of the set of zeros.

It follows immediately from (9.1) that $p_n(0) = a_0 = a_n \prod_{k=1}^{n} (-z_k)$. This shows that the absolute value of any zero of a polynomial must be finite. From (9.1), one readily verifies that

$$z^n p_n \left(\frac{1}{z} \right) = \sum_{k=0}^{n} a_{n-k} z^k = a_0 \prod_{k=1}^{n} \left(z - \frac{1}{z_k} \right) \tag{9.2}$$

Hence, the polynomial $\sum_{k=0}^{n} a_{n-k} z^k$ with the coefficients in reverse order possesses as zeros the inverses of those of the original polynomial $\sum_{k=0}^{n} a_k z^k$.

197. If all the coefficients a_k of $p_n(z) = \sum_{k=0}^{n} a_k x^k$ are integers and if $\xi = \frac{r}{s}$ is a rational zero (i.e. r and s are integers and coprime), then $r|a_0$ and $s|a_n$. Indeed, rewriting $p_n \left(\frac{r}{s} \right) = 0$ yields

$$r \sum_{k=0}^{n-1} a_{k+1} r^k s^{n-k-1} = -s^n a_0$$

which shows that r divides the left hand side and, hence, $r|s^n a_0$. Since the prime factorization of r and s do not have a prime number in common because r and s are coprime, $r|s^n a_0$ implies that $r|a_0$. The second statement follows analogously after rewriting $p_n \left(\frac{r}{s} \right) = 0$ as $a_n r^n = -s \sum_{k=0}^{n-1} a_k r^k s^{n-1-k}$. The zeros of a monic polynomial with integer coefficients are called algebraic numbers and play a fundamental role in algebraic number fields (see, e.g., Govers *et al.* (2008)).

198. The *Newton identities* for $0 \leq l < n$,

$$a_l = -\frac{1}{n-l} \sum_{k=l+1}^{n} a_k Z_{k-l} \tag{9.3}$$

derived in Van Mieghem (2006b, Appendix B.2), are a recursive set of equations that relate the coefficients a_k of a polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ to sums of positive powers $Z_j = \sum_{k=1}^{n} z_k^j$ of the zeros $z_1, z_2, \ldots, z_n$ of $p_n(z)$. An extension to the sum of negative powers follows from the same method and yields, for any $l < 0$,

$$Z_{-l} = -\frac{1}{a_0} \sum_{k=1}^{n} a_k Z_{k-l}$$

By rewriting the Newton identities as

$$Z_j = -\frac{1}{a_n} \left(j a_{n-j} + \sum_{k=1}^{j-1} a_{k+n-j} Z_k \right) \tag{9.4}$$

we obtain, for $1 \leq j \leq n$, a recursion that expresses the positive powers Z_j of the zeros in terms of the coefficients a_k. Explicitly for the first few Z_j,

$$Z_1 = \sum_{k=1}^{n} z_k = -\frac{a_{n-1}}{a_n} \tag{9.5}$$

$$Z_2 = \sum_{k=1}^{n} z_k^2 = \frac{a_{n-1}^2}{a_n^2} - \frac{2a_{n-2}}{a_n}$$

$$Z_3 = \sum_{k=1}^{n} z_k^3 = -\frac{a_{n-1}^3}{a_n^3} + \frac{3a_{n-2}a_{n-1}}{a_n^2} - \frac{3a_{n-3}}{a_n}$$

$$Z_4 = \sum_{k=1}^{n} z_k^4 = \frac{a_{n-1}^4}{a_n^4} - \frac{4a_{n-2}a_{n-1}^2}{a_n^3} + \frac{2a_{n-2}^2 + 4a_{n-3}a_{n-1}}{a_n^2} - 4\frac{a_{n-4}}{a_n}$$

Applying (9.5) to the polynomial $\sum_{k=0}^{n} a_{n-k} z^k$ with the coefficients in reverse order (**art. 196**) gives

$$Z_{-1} = \sum_{k=1}^{n} \frac{1}{z_k} = -\frac{a_1}{a_0}$$

$$Z_{-2} = \sum_{k=1}^{n} \frac{1}{z_k^2} = \frac{a_1^2}{a_0^2} - \frac{2a_2}{a_0}$$

If all zeros $\{z_k\}_{1 \leq k \leq n}$ are real and positive, the harmonic, geometric and arithmetic mean inequality (5.15) shows that

$$\frac{n}{Z_{-1}} \leq \sqrt[n]{\prod_{j=1}^{n} z_j} \leq \frac{1}{n} Z_1$$

from which we find $\frac{a_{n-1}}{a_n} \frac{a_1}{a_0} \geq n^2$.

199. *Vieta's formulae* express the coefficients a_k of $p_n(z)$ explicitly in terms of its zeros $\{z_k\}_{1\leq k\leq n}$.

Theorem 46 (Vieta) *For any polynomial defined by (9.1), it holds that, for $0 \leq k < n$,*

$$\frac{a_k}{a_n} = (-1)^{n-k} \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_{n-k}=j_{n-k-1}+1}^{n} \prod_{i=1}^{n-k} z_{j_i} \qquad (j_0 = 0) \qquad (9.6)$$

$$\equiv (-1)^{n-k} \sum_{1\leq j_1<j_2<\cdots<j_{n-k}\leq n} \prod_{i=1}^{n-k} z_{j_i} \qquad (9.7)$$

Proof: The proof is based on the principle of induction. Relation (9.6) is easily verified for $n = 2$. Assume that it holds for n. Consider now the polynomial of order $n + 1$ whose zeros are precisely those of $p_n(z)$, thus $z_k(n+1) = z_k(n)$ for $1 \leq k \leq n$ with the addition of the $n+1$ th zero, $z_{n+1}(n+1)$. Hence,

$$p_{n+1}(z) = (z - z_{n+1}(n+1))\, p_n(z)$$

$$= \sum_{k=1}^{n+1} a_{k-1}(n)\, z^k - \sum_{k=0}^{n} z_{n+1}(n+1)\, a_k(n)\, z^k$$

$$= -z_{n+1}(n+1)a_0(n) + \sum_{k=1}^{n}[a_{k-1}(n) - z_{n+1}(n+1)a_k(n)]z^k + a_n(n)z^{n+1}$$

from which the recursion

$$a_k(n+1) = a_{k-1}(n) - z_{n+1}(n+1)\, a_k(n)$$

is immediate. Since the coefficient of the highest power equals unity, by definition (thus $a_n(n) = a_{n+1}(n+1) = 1$) and since the constant term indeed reflects $(-1)^{n+1}$ times the product of all $n + 1$ zeros, we only have to verify the relation for the coefficients $a_k(n + 1)$ with $1 \leq k \leq n$, i.e., to check whether (9.6) satisfies the recursion relation. Substitution yields

$$a_k(n+1) = (-1)^{n+1-k} \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_{n+1-k}=j_{n-k}+1}^{n} \prod_{i=1}^{n+1-k} z_{j_i}(n)$$

$$- (-1)^{n-k} \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_{n-k}=j_{n-k-1}+1}^{n} \prod_{i=1}^{n-k} z_{j_i}(n)\, z_{n+1}(n+1)$$

Distributing the product of zeros over the sums and using $z_k(n + 1) = z_k(n)$ for

$1 \leq k \leq n$ leads to

$$a_k(n+1) = (-1)^{n+1\ k} \sum_{j_1=1}^{n} z_{j_1}(n+1) \sum_{j_2=j_1+1}^{n} z_{j_2}(n+1) \cdots \sum_{j_{n\ k}=j_{n\ k\ 1}+1}^{n} z_{j_{n\ k}}(n+1)$$

$$\left[\sum_{j_{n+1\ k}=j_{n\ k}+1}^{n} z_{j_{n+1\ k}}(n+1) + z_{n+1}(n+1) \right]$$

$$= (-1)^{n+1\ k} \sum_{j_1=1}^{n} z_{j_1}(n+1) \cdots \sum_{j_{n\ k}=j_{n\ k\ 1}+1}^{n} z_{j_{n\ k}}(n+1) \sum_{j_{n+1\ k}=j_{n\ k}+1}^{n+1} z_{j_{n+1\ k}}(n+1)$$

Since $\sum_{k=a}^{b} f(k) = 0$ if $a > b$, the last relation equals (9.6) when n is replaced by $n+1$. $\qquad\square$

In fact, this summation convention implies that (9.6) also equals

$$\frac{a_k}{a_n} = (-1)^{n\ k} \sum_{j_1=1}^{n\ k+1} \sum_{j_2=j_1+1}^{n\ k+2} \cdots \sum_{j_{n\ k}=j_{n\ k\ 1}+1}^{n} \prod_{i=1}^{k} z_{j_i} \tag{9.8}$$

In case for all k holds that $z_k(n) = 1$, we have $p_n(z) = (z-1)^n = \sum_{k=0}^{n} \binom{n}{k}(-1)^{n\ k} z^k$ from which the simple check

$$\sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_{n\ k}=j_{n\ k\ 1}+1}^{n} 1 = n\,(n-1)\cdots(n-k)/k! \equiv \binom{n}{k}$$

follows because only one ordering of $\{j_i\}$ out of $k!$ is allowed. Hence, the multiple sum in (9.6) consists of $\binom{n}{k}$ terms.

Applying (9.6) to (9.2) yields, after substitution of $m = n - k$, the following alternative expression:

$$a_m = (-1)^m a_0 \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_m=j_{m\ 1}+1}^{n} \prod_{i=1}^{m} \frac{1}{z_{j_i}} \tag{9.9}$$

Finally, if the multiplicity of the zeros is known, then the polynomial can be written as

$$p_n(z) = a_n \prod_{k=1}^{l} (z - z_k)^{m_k}$$

Using Newton's binomium $(z - z_k)^{m_k} = \sum_{j=0}^{m_k} \binom{m_k}{j} (-z_k)^j z^{m_k\ j}$, expansion of the product yields

$$p_n(z) = a_n \sum_{j_1=0}^{m_1} \binom{m_1}{j_1} (-z_1)^{j_1} \sum_{j_2=0}^{m_2} \binom{m_2}{j_2} (-z_2)^{j_2} \ldots \sum_{j_l=0}^{m_l} \binom{m_l}{j_l} (-z_l)^{j_l} z^{n\ \sum_{k\ 1}^{l} j_k}$$

where we have used $\sum_{k=1}^{l} m_l = n$ (**art. 196**). Let $q = \sum_{k=1}^{l} j_l$, then

$$p_n(z) = (-1)^n a_n \sum_{q=0}^{n} \left\{ \sum_{\sum_{k}^{l} 1 j_k = q; j_k \geq 0} \prod_{k=1}^{l} \binom{m_k}{j_k} (-z_k)^{j_k} \right\} z^q$$

from which the coefficient a_q follows as

$$a_q = (-1)^{n-q} a_n \sum_{\sum_{k}^{l} 1 j_k = q; j_k \geq 0} \prod_{k=1}^{l} \binom{m_k}{j_k} z_k^{j_k}$$

The last sum is an instance of a characteristic coefficient of complex function, first defined in Van Mieghem (1996).

200. The *elementary symmetric polynomials* of degree k in n variables $z_1, z_2, \ldots, z_n$ are defined by

$$e_k(z_1, z_2, \ldots, z_n) = (-1)^{n-k} \frac{a_{n-k}}{a_n}$$

where $\frac{a_{n-k}}{a_n}$ is given in either (9.6) or (9.7). For example, for $n = 1$,

$$e_1(z_1) = z_1$$

for $n = 2$,

$$e_1(z_1, z_2) = z_1 + z_2$$
$$e_2(z_1, z_2) = z_1 z_2$$

for $n = 3$,

$$e_1(z_1, z_2, z_3) = z_1 + z_2 + z_3$$
$$e_2(z_1, z_2, z_3) = z_1 z_2 + z_1 z_3 + z_2 z_3$$
$$e_3(z_1, z_2, z_3) = z_1 z_2 z_3$$

for $n = 4$,

$$e_1(z_1, z_2, z_3, z_4) = z_1 + z_2 + z_3 + z_4$$
$$e_2(z_1, z_2, z_3, z_4) = z_1 z_2 + z_1 z_3 + z_1 z_4 + z_2 z_3 + z_2 z_4 + z_3 z_4$$
$$e_3(z_1, z_2, z_3, z_4) = z_1 z_2 z_3 + z_1 z_2 z_4 + z_1 z_3 z_4 + z_2 z_3 z_4$$
$$e_4(z_1, z_2, z_3, z_4) = z_1 z_2 z_3 z_4$$

For each positive integer $k \leq n$, there exists exactly one elementary symmetric polynomial of degree k in n variables, which is formed by the sum of all different products of k tuples of the n variables. Since each such a product $\prod_{j=1}^{k} z_j$ is commutative, all linear combinations of products of the elementary symmetric polynomials constitute a commutative ring, which lies at the basis of Galois theory. For example, it can be shown that any symmetric polynomial in n variables can be expressed in a unique way in terms of the elementary symmetric polynomials $e_k(z_1, z_2, \ldots, z_n)$ for $1 \leq k \leq n$.

201. *Discriminant of a polynomial.* The discriminant of a polynomial $p_n(z)$ is defined for $n \geq 2$ as

$$\Delta(p_n) = a_n^{2n-2} \prod_{1 \leq k < j \leq n} (z_j - z_k)^2 \tag{9.10}$$

with the convention that $\Delta(p_1) = 1$. In view of (8.92), the discriminant can be written in terms of the Vandermonde determinant as

$$\Delta(p_n) = a_n^{2n-2} (\det V_n(z))^2 \tag{9.11}$$

where $z = (z_1, z_2, \ldots, z_n)$ is the vector of the zeros of $p_n(z)$. The definition (9.10) of the discriminant shows that $\Delta(p_n) = 0$ when, at least one zero has a multiplicity larger than 1. In order words, $\Delta(p_n) \neq 0$ if and only if all zeros of $p_n(z)$ are simple or distinct.

Since the discriminant is a symmetric polynomial in the zeros and any symmetric polynomial can be expressed in a unique way in terms of the elementary symmetric polynomials (**art.** 200), the discriminant can also be expressed in terms of the coefficients of the polynomial. For example, for $n = 2$, we obtain the well known discriminant of the quadratic polynomial $p_2(z) = az^2 + bz + c$ as

$$\Delta(p_2) = b^2 - 4ac$$

The discriminant of the cubic $p_3(z) = az^3 + bz^2 + cz + d$ is

$$\Delta(p_3) = b^2 c^2 - 4ac^3 - 4b^3 d - 27a^2 d^2 + 18abcd$$

202. *Discriminant and the derivative of a polynomial.* The logarithmic derivative of $p_n(z)$, defined in (9.1), is

$$\frac{d \log p_n(z)}{dz} = \frac{p_n'(z)}{p_n(z)} = \sum_{k=1}^{n} \frac{1}{z - z_k}$$

which shows that

$$p_n'(z) = a_n \sum_{k=1}^{n} \prod_{j=1; j \neq k}^{n} (z - z_j)$$

Evaluated at a zero z_m of $p_n(z)$ gives

$$p_n'(z_m) = a_n \prod_{j=1; j \neq m}^{n} (z_m - z_j) = a_n (-1)^{m-1} \prod_{j=1; j \neq m}^{m-1} (z_j - z_m) \prod_{j=m+1}^{n} (z_m - z_j)$$

from which we obtain

$$\prod_{m=1}^{n} p_n'(z_m) = a_n^n (-1)^{\frac{n(n-1)}{2}} \prod_{m=1}^{n} \prod_{j=m+1}^{n} (z_j - z_m)^2$$

By invoking the definition (9.10) of the discriminant, we arrive at

$$\Delta(p_n) = (-1)^{\frac{n(n-1)}{2}} a_n^{n-2} \prod_{m=1}^{n} p_n'(z_m) \tag{9.12}$$

which shows that, if the discriminant is non zero, the derivative $p_n'(z)$ has all its zeros different from the simple zeros of $p_n(z)$. In cases where a differential equation for a set of polynomials is known, such as for most classical orthogonal polynomials, the relation (9.12) can be used to express the discriminant in closed form as shown in Milovanović *et al.* (1994, p. 67).

9.2 Transforming polynomials

203. Any polynomial

$$q_n(z) = \sum_{j=0}^{n} b_j z^j = b_n \prod_{k=1}^{n} (z - y_k)$$

where $b_n \neq 0$ can be reduced by a linear transformation $z = x + c$ into a polynomial $p_n(x) = \sum_{k=0}^{n} a_k x^k$, where the coefficient a_{n-1} of x^{n-1} is zero. Indeed,

$$q_n(x+c) = \sum_{j=0}^{n} b_j (x+c)^j = \sum_{j=0}^{n} b_j \sum_{k=0}^{j} \binom{j}{k} x^k c^{j-k}$$

$$= \sum_{k=0}^{n} \left(\sum_{j=k}^{n} b_j \binom{j}{k} c^{j-k} \right) x^k$$

$$= b_n x^n + (b_{n-1} + n b_n c) x^{n-1} + \ldots + \sum_{j=0}^{n} b_j c^j$$

which shows that, if $c = -\frac{b_{n-1}}{n b_n}$, the polynomial $p_n(x) = q_n(x+c)$ possesses a zero coefficient of x^{n-1}, thus $a_{n-1} = 0$. Clearly, a linear transform shifts the zeros $\{y_k\}_{1 \leq k \leq n}$ of $q_n(z)$ to the zeros $\{y_k - c\}_{1 \leq k \leq n}$ of $p_n(z)$. The sum of zeros of $p_n(z)$ is zero by (9.5) such that c is the mean of the zeros of $q_n(z)$. Hence, without loss of generality, any polynomial $q_n(z)$ can be first transformed by $z = x + c$ with $c = -\frac{b_{n-1}}{n b_n}$ into the polynomial $p_n(x)$, where $a_k = \sum_{j=k}^{n} b_j \binom{j}{k} c^{j-k}$ and $a_{n-1} = 0$.

The Newton identity $Z_2 = \sum_{k=1}^{n} (y_k - c)^2 = -\frac{2 a_{n-2}}{a_n}$ shows that the (real) coefficients a_{n-2} and a_n of a polynomial $p_n(x)$, where $a_{n-1} = 0$ must have opposite sign if all zeros are real.

204. The conformal mapping $w = \frac{1-z}{1+z}$ and $z = \frac{1-w}{1+w}$ transforms the right half complex plane $\text{Re}(z) > 0$ into the unit circle $|w| < 1$. For, let $z = r e^{i\theta}$, then

$$w = \frac{1 - e^{i\theta + \ln r}}{1 + e^{i\theta + \ln r}} = \frac{e^{\frac{i\theta + \ln r}{2}} \left(e^{-\frac{i\theta + \ln r}{2}} - e^{\frac{i\theta + \ln r}{2}} \right)}{e^{\frac{i\theta + \ln r}{2}} \left(e^{-\frac{i\theta + \ln r}{2}} + e^{\frac{i\theta + \ln r}{2}} \right)} = -\tanh\left(\frac{\ln r + i\theta}{2} \right)$$

which can also be written as

$$w = \sqrt{\frac{\cosh \ln r - \cos \theta}{\cosh \ln r + \cos \theta}} e^{i\left(\arctan\left(\frac{\sin \theta}{\sinh \ln r}\right) + \pi\right)}$$

If $r = 1$, then $w = i \tan \frac{\theta}{2}$, which shows that a point z on the unit circle is mapped into a point w on the imaginary axis (and vice versa). If $\mathrm{Re}\,(z) < 0$ or $\theta \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right)$, then $\cos \theta < 0$ and $|w| = \sqrt{\frac{\cosh \ln r \ \cos \theta}{\cosh \ln r + \cos \theta}} > 1$, while, if $\mathrm{Re}\,(z) > 0$ or $\theta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ and $\cos \theta > 0$, then $|w| < 1$.

If all zeros of $p_n\,(-z)$ lie in the left half complex plane (similarly, all zeros of $p_n\,(z)$ lie in the $\mathrm{Re}\,(z) > 0$ plane), then all zeros of $p_n\left(\frac{1-w}{1+w}\right)$ lie inside the unit circle $|w| < 1$. The function[1]

$$p_n\left(\frac{1-w}{1+w}\right) = (1+w)^{-n} \sum_{k=0}^{n} a_k\,(1+w)^{n\ k}\,(1-w)^k$$

has the same (finite) zeros as the polynomial

$$q_n\,(w) = \sum_{k=0}^{n} a_k\,(1+w)^{n\ k}\,(1-w)^k$$

Using Newton's binomium and the Cauchy product, gives

$$(1+w)^{n\ k}\,(1-w)^k = \sum_{m=0}^{n} \sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j} w^m$$

such that $q_n\,(w) = \sum_{m=0}^{n} b_m w^m$, where

$$b_m = \sum_{j=0}^{m}(-1)^j \sum_{k=0}^{n} a_k\,\binom{k}{j}\binom{n-k}{m-j}$$

$$= \sum_{k=0}^{n} B_{mk} a_k$$

Defining the matrix elements $B_{mk} = \sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n\ k}{m\ j}$ of the $(n+1) \times (n+1)$ matrix B, we can write the coefficient vector b in terms of the coefficient vector a as $b = Ba$. Since, $q_n\,(1) = a_0\,2^n$, which is, for any set of coefficients a_k, equivalent to

$$\sum_{m=0}^{n} b_m = \sum_{m=0}^{n} \sum_{j=0}^{m}(-1)^j \sum_{k=0}^{n} a_k\,\binom{k}{j}\binom{n-k}{m-j} = 2^n a_0$$

we find, by equating corresponding coefficients a_k that

$$\sum_{m=0}^{n} \sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j} = 2^n 1_{\{k=0\}} = \sum_{m=0}^{n} B_{mk}$$

---

[1] Notice $p_n\left(\frac{1-w}{1+w}\right)$ has all zeros outside the unit circle and that $w^n q_n\,(w^{-1})$ $\sum_{m\ 0}^{n}\left(\sum_{j\ 0}^{m}(\ 1)^j \sum_{k\ 0}^{n} a_k\,(\ 1)^k \binom{k}{j}\binom{n-k}{m-j}\right) w^m$.

Hence, the sums over the rows of B are zero, except for the zeroth column $k = 0$.

Let us consider the inverse transform $w = \frac{1-z}{1+z}$. From $p_n\left(\frac{1}{1+w}\right) = (1+w)^{-n} q_n(w)$, we have that

$$p_n(z) = 2^{-n}(1+z)^n q_n\left(\frac{1-z}{1+z}\right)$$

On the other hand,

$$q_n\left(\frac{1-z}{1+z}\right) = \sum_{m=0}^{n} b_m \left(\frac{1-z}{1+z}\right)^m = (1+z)^{-n} \sum_{m=0}^{n} b_m (1+z)^{n-m}(1-z)^m$$

$$= (1+z)^{-n} \sum_{m=0}^{n} c_m z^m$$

where, since $b_k = \sum_{l=0}^{k}(-1)^l \sum_{q=0}^{n} a_q \binom{q}{l}\binom{n}{k}\binom{q}{l}$,

$$c_m = \sum_{j=0}^{m}(-1)^j \sum_{k=0}^{n} b_k \binom{k}{j}\binom{n-k}{m-j}$$

$$= \sum_{j=0}^{m}(-1)^j \sum_{k=0}^{n} \left(\sum_{l=0}^{k}(-1)^l \sum_{q=0}^{n} a_q \binom{q}{l}\binom{n-q}{k-l}\right) \binom{k}{j}\binom{n-k}{m-j}$$

$$= \sum_{q=0}^{n} a_q \sum_{k=0}^{n} \left(\sum_{l=0}^{k}(-1)^l \binom{q}{l}\binom{n-q}{k-l}\right) \left(\sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j}\right)$$

Thus, $p_n(z) = 2^{-n} \sum_{m=0}^{n} c_m z^m$ and since $p_n(z) = \sum_{m=0}^{n} a_m z^m$, we must have that

$$a_m = 2^{-n} c_m$$

$$= 2^{-n} \sum_{q=0}^{n} a_q \sum_{k=0}^{n} \left(\sum_{l=0}^{k}(-1)^l \binom{q}{l}\binom{n-q}{k-l}\right) \left(\sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j}\right)$$

or, after equating corresponding coefficients a_m,

$$\sum_{k=0}^{n} \left(\sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j}\right) \left(\sum_{l=0}^{k}(-1)^l \binom{q}{l}\binom{n-q}{k-l}\right) = 2^n \delta_{qm}$$

In terms of the matrix elements $B_{mk} = \sum_{j=0}^{m}(-1)^j \binom{k}{j}\binom{n-k}{m-j}$, we observe that

$$\sum_{k=0}^{n} B_{mk} B_{kq} = 2^n \delta_{qm}$$

Hence, the matrix $B^2 = 2^n I$.

If all zeros of $q_n(w)$ lie inside the unit circle, then the sequence of the power sums

$Z_j = \sum_{k=1}^{n} z_k^j$ is strictly decreasing in j. **Art. 229** below gives another check. In addition, the sum of the inverses of the zeros $w_1, w_2, \ldots, w_n$ of $q_n(w)$ is (**art. 198**)

$$\sum_{k=1}^{n} \frac{1}{w_k} = -\frac{b_1}{b_0} = -\frac{\sum_{k=0}^{n}(n-2k)a_k}{\sum_{k=0}^{n} a_k}$$

$$= -\frac{\frac{d}{dw}(1+w)^n p_n\left(\frac{1}{1+w}\frac{w}{}\right)\Big|_{w=0}}{p_n(1)} = -n + \frac{2p_n'(1)}{p_n(1)}$$

205. Consider an even polynomial $r_{2n}(z) = \sum_{k=0}^{n} a_{2k} z^{2k}$. Conformal mapping $w = \frac{1-z}{1+z}$ and $z = \frac{1-w}{1+w}$ leads to

$$r_{2n}\left(\frac{1-w}{1+w}\right) = (1+w)^{-2n} \sum_{k=0}^{n} a_{2k}(1+w)^{2n-2k}(1-w)^{2k} = r_{2n}\left(-\frac{1-w}{1+w}\right)$$

$$= (1+w)^{-2n} t_{2n}(w)$$

where

$$t_{2n}(w) = \sum_{m=0}^{2n} b_m^* w^m$$

and

$$b_m^* = \sum_{j=0}^{m}(-1)^j \sum_{k=0}^{n} a_{2k}\binom{2k}{j}\binom{2n-2k}{m-j}$$

The inverse transform $w = \frac{1-z}{1+z}$ applied to $r_{2n}\left(\frac{1-w}{1+w}\right) = (1+w)^{-2n} t_{2n}(w)$ gives

$$r_{2n}(z) = 2^{-2n}(1+z)^{2n} t_{2n}\left(\frac{1-z}{1+z}\right) = 2^{-2n}(1-z)^{2n} t_{2n}\left(\frac{1+z}{1-z}\right)$$

where the latter follows from $r_{2n}(z) = r_{2n}(-z)$. Explicitly, we have that

$$(1+z)^{2n} t_{2n}\left(\frac{1-z}{1+z}\right) = \sum_{m=0}^{2n} b_m^* (1-z)^m (1+z)^{2n-m}$$

and

$$(1-z)^{2n} t_{2n}\left(\frac{1+z}{1-z}\right) = \sum_{m=0}^{2n} b_m^* (1-z)^{2n-m}(1+z)^m$$

$$= \sum_{q=0}^{2n} b_{2n-m}^* (1-z)^q (1+z)^{2n-q}$$

Equating corresponding powers in $(1-z)^m (1+z)^m = (1-z^2)^m$ shows that

$$b_m^* = b_{2n-m}^*$$

Hence, the coefficients b_m^* are symmetric around b_n^*. Thus,

$$w^{2n} t_{2n}\left(\frac{1}{w}\right) = \sum_{m=0}^{2n} b_m^* w^{2n-m} = \sum_{m=0}^{2n} b_{2n-m}^* w^{2n-m} = \sum_{q=0}^{2n} b_q^* w^q = t_{2n}(w)$$

or, in symmetric form[2], $w^n t_{2n}\left(\frac{1}{w}\right) = w^{-n} t_{2n}(w)$. This shows that, if the polynomial $t_{2n}(w)$ does not have a zero inside (and thus also outside) the unit circle, all $2n$ zeros of $t_{2n}(w)$ must lie on the unit circle, which is equivalent to the fact that all zeros of $r_{2n}(z)$ lie on the imaginary axis.

On the other hand, we can write

$$t_{2n}(w) = \sum_{m=0}^{n} b_m^* w^m + \sum_{m=n+1}^{2n} b_{2n-m}^* w^m$$

$$= \sum_{m=0}^{n-1} b_m^* w^m + b_n^* w^n + \sum_{m=0}^{n-1} b_m^* w^{2n-m}$$

$$= w^n \left(b_n^* + \sum_{m=0}^{n-1} b_m^* \left(w^{m-n} + w^{n-m} \right) \right)$$

Let $w = re^{i\theta}$, then with $w^{m-n} + w^{n-m} = 2\cosh((n-m)(\ln r + i\theta))$, we have

$$w^{-n} t_{2n}(w) = b_n^* + 2\sum_{k=1}^{n} b_{n+k}^* \cosh(k(\ln r + i\theta))$$

If $r = 1$, and if $b_n^* < 2b_{n+1}^* < 2b_{n+2}^* < \cdots < 2b_{2n}^*$ then

$$e^{-in\theta} t_{2n}\left(e^{i\theta}\right) = b_n^* + 2\sum_{k=1}^{n} b_{n+k}^* \cos(k\theta)$$

has $2n$ distinct real roots in the interval $0 < \theta < 2\pi$, and no imaginary roots at all. The proof is given in Markushevich (1985, Vol. II, pp. 50–52).

9.3 Interpolation

206. *Lagrange interpolation.* Interpolation consists of constructing a polynomial that passes through at set of n distinct points, defined by their finite coordinates (x_j, y_j) for $1 \le j \le n$. In many cases, the ordinates are special instances of a function, $y_j = f(x_j)$, that we want to approximate by a polynomial. Lagrange has developed a most convenient way to construct this "interpolating" polynomial.

We start considering the polynomial of degree n,

$$F_n(x) = \prod_{j=1}^{n} (x - x_j) \tag{9.13}$$

---

[2] Polynomials $p_n(z)$ with complex coefficients that satisfy $\sum_{k=0}^{n} a_k z^k = \sum_{k=0}^{n} (a_{n-k})^* z^k$, equivalent to $p_n(z) = (z^n p_n(z^{-1}))^*$ are called self-inversive and discussed in Sheil-Small (2002, Chapter 7).

Clearly, $\frac{F_n(x)}{x-x_k} = \prod_{j=1;j\neq k}^{n}(x-x_j)$ is a polynomial of degree $n-1$ and, since $F_n(x_k) = 0$, we have that

$$\lim_{x\to x_k}\frac{F_n(x)}{x-x_k} = \lim_{x\to x_k}\frac{F_n(x)-F_n(x_k)}{x-x_k} = F_n'(x_k) = \prod_{j=1;j\neq k}^{n}(x_k-x_j) \qquad (9.14)$$

Since all x_k are distinct, x_k is a simple zero of $F_n(x)$ such that $F_n'(x_k) \neq 0$. Hence, the polynomial of degree $n-1$,

$$l_{n-1}(x;x_k) = \frac{F_n(x)}{(x-x_k)F_n'(x_k)} = \prod_{j=1;j\neq k}^{n}\frac{x-x_j}{x_k-x_j} \qquad (9.15)$$

possesses the interesting property that, at any of the abscissa $x_1, x_2, \ldots, x_n$, it vanishes, except at $x = x_k$, where it is one. Thus, with the "Kronecker's delta" δ_{kj}, which is defined as $\delta_{kj} = 0$ if $j \neq k$, and $\delta_{kk} = 1$, it holds that

$$l_{n-1}(x_j;x_k) = \delta_{kj}$$

Lagrange observed that the polynomial of degree $n-1$,

$$p_{n-1}(x) = \sum_{j=1}^{n} y_j l_{n-1}(x;x_j) \qquad (9.16)$$

passes through all n points $\{(x_j, y_j)\}_{1\leq j\leq n}$, with $y_j = p_{n-1}(x_j)$ for $1 \leq j \leq n$. The polynomial (9.16) is called the Lagrange interpolation polynomial corresponding to the set of n points $\{(x_j, y_j)\}_{1\leq j\leq n}$.

The Lagrange polynomial (9.16) is unique. Indeed, assume that there is another polynomial $q_{n-1}(x)$ that passes through the same set of n points. Then $p_{n-1}(x) - q_{n-1}(x)$ is again a polynomial of degree $n-1$ that possesses n zeros at x_j for $1 \leq j \leq n$, which is impossible (**art. 196**). Hence, $p_{n-1}(x) = q_{n-1}(x)$, which establishes the uniqueness.

207. *Newton interpolation.* When the set of abscissa $\{x_k\}_{1\leq k\leq n}$ is chosen in an equidistant way as $x_k = k\Delta x$ for $1 \leq k \leq n$, then the Lagrange interpolating polynomial (9.16) reduces to

$$p_{n-1}(x) = F_n(x) \sum_{j=1}^{n} \frac{p_{n-1}(j\Delta x)}{(x-j\Delta x) \prod_{m=1;m\neq j}^{n}(j-m)\Delta x}$$

Using $\prod_{m=1;m\neq j}^{n}(j-m) = (-1)^{n-j}(j-1)!(n-j)!$, we obtain a variant of Newton's interpolating polynomial,

$$p_{n-1}(x) = \frac{\prod_{k=1}^{n}(x-k\Delta x)}{(\Delta x)^{n-1}(n-1)!} \sum_{j=1}^{n}\binom{n-1}{j-1}\frac{(-1)^{n-j}p_{n-1}(j\Delta x)}{x-j\Delta x}$$

It is often more convenient to interpolate the polynomial $p_n(x)$ from $x_1 = 0$ with steps of $\Delta x = y$ up to $x_n = (n-1)y$, in which case we arrive at the classical Newton interpolating polynomial:

$$p_n(xy) = \frac{\prod\limits_{k=0}^{n}(x-k)}{n!} \sum_{j=0}^{n}\binom{n}{j}\frac{(-1)^{n\ j}\,p_n(jy)}{x-j} \tag{9.17}$$

In particular, the special case where $x = -1$ leads to

$$p_n(-y) = \sum_{j=0}^{n}\binom{n+1}{j+1}(-1)^j\,p_n(jy) \tag{9.18}$$

which expresses the negative argument values of a polynomial in terms of positive argument values.

Finally, we present

$$p_n(xy) = \sum_{q=0}^{n}\Delta^q p_n(qx)\binom{y}{q} \tag{9.19}$$

where

$$\Delta^q p_n(qx) = \sum_{k=0}^{q}(-1)^{q\ k}\binom{q}{k}p_n(kx)$$

is the q th difference obeying $\Delta^q f_m = \Delta^{q\ 1}f_{m+1} - \Delta^{q\ 1}f_m$ for all $q \in \mathbb{N}_0$, thus $\Delta f_m = f_{m+1} - f_m$. By iteration, we have that $\Delta^q f_m = \sum_{k=0}^{q}\binom{q}{k}(-1)^{q\ k}f_{m\ q+k}$. Substituting the polynomial form, $p_n(x) = \sum_{k=0}^{n}a_k x^k$ into the q th difference yields

$$\frac{\Delta^q p_n(qx)}{q!} = \sum_{m=q}^{n}\mathcal{S}_m^{(q)}a_m x^m$$

where $\mathcal{S}_m^{(q)}$ are the Stirling Numbers of the Second Kind (Abramowitz and Stegun, 1968, Section 24.1.4). The relation (9.19) is commonly known for $x = 1$ as Newton's difference expansion for polynomials. If both sides of (9.19) converge in the limit for $n \to \infty$, the left hand side converges to the Taylor series of a complex function f, and the right hand side then equals the difference expansion for f. Using the formula

$$\sum_{j=k}^{n}(-1)^{k+j}\binom{j}{k}\binom{y}{j} = \frac{(-1)^{k+n}\,\Gamma(1+y)}{(y-k)\,k!(n-k)!\,\Gamma(-n+y)} \tag{9.20}$$

$$= \delta_{n,k} \qquad\qquad \text{if } y = n$$

where $\Gamma(x)$ is the Gamma function, we may verify that Newton's difference expansion (9.19) for polynomials is equivalent to Newton's interpolating formula (9.17).

9.4 The Euclidean algorithm

208. Consider two polynomials[3] $p_0(z) = \sum_{k=0}^{n} a_k z^k$ and $p_1(z) = \sum_{k=0}^{m} b_k z^k$, both with complex coefficients and where the degree n of $p_0(z)$ is larger than or equal to m. Then, there always exists a polynomial $q_1(z)$, called the quotient, such that

$$p_0(z) = q_1(z) p_1(z) + p_2(z)$$

and the degree of the remainder polynomial $p_2(z)$ is smaller than m. Indeed, we can always remove the highest degree term $a_n z^n$ in $p_0(z)$ by subtracting $\frac{a_n}{b_m} z^{n\ m} p_1(z)$. This first step in the long division yields

$$p_0(z) - \frac{a_n}{b_m} z^{n\ m} p_1(z) = \sum_{j=0}^{n\ 1} \left(a_j - \frac{a_n}{b_m} b_{j\ n+m} \right) z^j = r(z)$$

where the convention $b_{\ j} = 0$ for $j > 0$ and where the degree of $r(z) = \sum_{j=0}^{n\ 1} r_j z^j$ is at most $n-1$. If the degree of the remainder $r(z)$ is larger than m, we repeat the process and subtract $\frac{r_{n\ 1}}{b_m} z^{n\ 1\ m} p_1(z)$ from $r(z)$, resulting in a remainder with degree at most $n-2$. As long as the degree of the remainder polynomial exceeds m, we repeat the process of subsequent lowering the highest degree. Eventually, we arrive at a remainder $p_2(z)$ with degree smaller than m. This operation is the well known long division.

Next, we can rewrite the equation as

$$\frac{p_0(z)}{p_1(z)} = q_1(z) + \frac{p_2(z)}{p_1(z)} = q_1(z) + \frac{1}{\frac{p_1(z)}{p_2(z)}}$$

and apply the same recipe to $\frac{p_1(z)}{p_2(z)} = q_2(z) + \frac{p_3(z)}{p_2(z)}$, where the degree of $p_3(z)$ is smaller than that of $p_2(z)$. Thus,

$$\frac{p_0(z)}{p_1(z)} = q_1(z) + \frac{1}{q_2(z) + \frac{1}{\frac{p_2(z)}{p_3(z)}}}$$

We can repeat the recipe to $\frac{p_2(z)}{p_3(z)} = q_3(z) + \frac{p_4(z)}{p_3(z)}$, where again the degree of $p_4(z)$ is smaller than that of $p_3(z)$. Hence, we can always reduce the degree of the remainder and eventually it will be equal to zero. The result is a finite continued fraction for $\frac{p_0(z)}{p_1(z)}$ in terms of the subsequent quotients $q_1(z), q_2(z), \ldots, q_m(z)$,

$$\frac{p_0(z)}{p_1(z)} = q_1(z) + \cfrac{1}{q_2(z) + \cfrac{1}{q_3(z) + \cfrac{1}{\ddots + \cfrac{1}{q_m(z)}}}}$$

---

[3] The index n in p_n here deviates from the general definition (9.1).

Alternatively, we obtain a system of polynomial equations

$$
\begin{array}{ll}
p_0(z) = q_1(z)\,p_1(z) + p_2(z) & (0 < \deg p_2 < \deg p_1) \\
p_1(z) = q_2(z)\,p_2(z) + p_3(z) & (0 < \deg p_3 < \deg p_2) \\
p_2(z) = q_3(z)\,p_3(z) + p_4(z) & (0 < \deg p_4 < \deg p_3) \\
\cdots & \cdots \\
p_{m-2}(z) = q_{m-1}(z)\,p_{m-1}(z) + p_m(z) & (0 < \deg p_m < \deg p_{m-1}) \\
p_{m-1}(z) = q_m(z)\,p_m(z)
\end{array}
$$

which is known as Euclid's algorithm. The last equation shows that $p_m(z)$ divides $p_{m-1}(z)$. The last but one polynomial equation indicates that $p_m(z)$ also divides $p_{m-2}(z)$. Continuing upwards, we see that the polynomial $p_m(z)$ divides all polynomials $p_k(z)$ with $0 \le k \le m$. Hence, $p_m(z)$ cannot be zero for all z, otherwise all $p_k(z)$ would be zero.

Also, $p_m(z)$ is the largest common divisor polynomial[4] of both $p_0(z)$ and $p_1(z)$. Indeed, any divisor polynomial $d(z)$ of $p_0(z)$ and $p_1(z)$ obeys $d|p_0$ and $d|p_1$, then the first Euclidean equation indicates that $d|p_2$, and subsequently, $d|p_k$. Since the degree of the sequence of polynomials $p_k(z)$ strictly decreases, $p_m(z)$ is the largest possible common divisor polynomial. Consequently, the functions $f_k(z) = \frac{p_k(z)}{p_m(z)}$ are again polynomials.

209. *Division by a first degree polynomial.* The division of $p_0(z) = \sum_{k=0}^n a_k z^k$ by $p_1(z) = z - \xi$ can be computed explicitly. The long division of $p_0(z)$ by $z - \xi$ gives the remainder $p_2(z) = p_0(\xi)$ and the quotient

$$
q_1(z) = \sum_{k=0}^{n-1} \left\{ \frac{1}{\xi^{k+1}} \sum_{j=k+1}^{n} a_j \xi^j \right\} z^k \tag{9.21}
$$

It is instructive to relate the long division with Taylor series expansions in analysis. With the convention that $a_k = 0$ if $k > n$, execution of the Cauchy product of two Taylor series around $z = 0$ yields, for $|z| < |\xi|$,

$$
\frac{p_0(z)}{z - \xi} = -\sum_{k=0}^{\infty} a_k z^k \sum_{k=0}^{\infty} \frac{z^k}{\xi^{k+1}} = -\sum_{k=0}^{\infty} \left\{ \frac{1}{\xi^{k+1}} \sum_{j=0}^{k} a_j \xi^j \right\} z^k
$$

We split the series into two parts and take into account that $a_k = 0$ if $k > n$,

$$
\frac{p_0(z)}{z - \xi} = -\sum_{k=0}^{n-1} \left\{ \frac{1}{\xi^{k+1}} \sum_{j=0}^{k} a_j \xi^j \right\} z^k - \sum_{k=n}^{\infty} \left\{ \frac{1}{\xi^{k+1}} \sum_{j=0}^{n} a_j \xi^j \right\} z^k
$$

---

[4] For a particular value of $z = z_0$, we obtain the greatest common divisor of the two numbers $p_0(z_0)$ and $p_1(z_0)$.

Observing that $p_0(\xi) = \sum_{j=0}^{n} a_j \xi^j$, the last sum equals

$$\sum_{k=n}^{\infty} \left\{ \frac{1}{\xi^{k+1}} \sum_{j=0}^{n} a_j \xi^j \right\} z^k = p_0(\xi) \sum_{k=n}^{\infty} \frac{z^k}{\xi^{k+1}} = p_0(\xi) \left(\sum_{k=0}^{\infty} \frac{z^k}{\xi^{k+1}} - \sum_{k=0}^{n-1} \frac{z^k}{\xi^{k+1}} \right)$$

$$= -\frac{p_0(\xi)}{z - \xi} - p_0(\xi) \sum_{k=0}^{n-1} \frac{z^k}{\xi^{k+1}}$$

such that

$$\frac{p_0(z)}{z - \xi} = \sum_{k=0}^{n-1} \left\{ \frac{1}{\xi^{k+1}} \left(p_0(\xi) - \sum_{j=0}^{k} a_j \xi^j \right) \right\} z^k + \frac{p_0(\xi)}{z - \xi} \tag{9.22}$$

where the sum equals is the quotient $q_1(z)$ in (9.21) obtained by the long division. Hence, we obtain the difference quotient

$$q_1(z) = \frac{p_0(z) - p_0(\xi)}{z - \xi}$$

from which it follows that $q_1(\xi) = p_0'(\xi)$. The latter is, indeed, deduced from (9.21) as

$$q_1(\xi) = \sum_{k=0}^{n-1} \sum_{j=k}^{n-1} a_{j+1} \xi^j = \sum_{j=0}^{n-1} a_{j+1} \xi^j \sum_{k=0}^{j} 1 = \sum_{j=0}^{n-1} (j+1) a_{j+1} \xi^j = p_0'(\xi)$$

The case, in which ξ is a zero of $p_0(z)$, is of particular interest,

$$\frac{p_0(z)}{z - \xi} = \sum_{k=0}^{n-1} \left\{ \frac{1}{\xi^{k+1}} \left(\sum_{j=k+1}^{n} a_j \xi^j \right) \right\} z^k = -\sum_{k=0}^{n-1} \left\{ \frac{1}{\xi^{k+1}} \left(\sum_{j=0}^{k} a_j \xi^j \right) \right\} z^k$$

This expression gives the explicit quotient polynomial $q_1(z)$ after division by a linear factor $z - \xi$ where $p_0(\xi) = 0$.

210. *Division by a m degree polynomial.* By using the Taylor series in case $m = 2$,

$$\frac{1}{(z - \xi)(z - \zeta)} = \frac{1}{\xi \zeta} \sum_{k=0}^{\infty} \frac{z^k}{\xi^k} \sum_{k=0}^{\infty} \frac{z^k}{\zeta^k} = \frac{1}{\xi \zeta} \sum_{k=0}^{\infty} \left\{ \frac{1}{\zeta^k} \sum_{j=0}^{k} \left(\frac{\zeta}{\xi} \right)^j \right\} z^k$$

$$= \frac{1}{\xi - \zeta} \sum_{k=0}^{\infty} \left(\frac{1}{\zeta^{k+1}} - \frac{1}{\xi^{k+1}} \right) z^k$$

a similar series expansion manipulation as in **art. 209** leads to

$$\frac{p_0(z)}{(z - \xi)(z - \zeta)} = \frac{1}{\zeta - \xi} \sum_{k=0}^{n-2} \left\{ \frac{1}{\zeta^{k+1}} \sum_{j=k+1}^{n} a_j \zeta^j - \frac{1}{\xi^{k+1}} \sum_{j=k+1}^{n} a_j \xi^j \right\} z^k$$

$$+ \frac{p_0(\zeta)}{\zeta - \xi} \frac{1}{z - \zeta} + \frac{p_0(\xi)}{\xi - \zeta} \frac{1}{z - \xi}$$

When $\xi = \zeta$, differentiation yields

$$\frac{p_0(z)}{(z-\xi)^2} = \sum_{k=0}^{n-2} \left\{ \frac{1}{\zeta^{k+2}} \sum_{j=k+1}^{n} (j-k-1) a_j \zeta^j \right\} z^k + \frac{p_0'(\xi)}{z-\xi} + \frac{p_0(\xi)}{(z-\xi)^2}$$

The general result is most elegantly deduced from Cauchy's integral theorem,

$$f(z) = \frac{1}{2\pi i} \int_{C(z)} \frac{f(w)}{w-z} dw$$

where the contour $C(z)$ encloses the point $w = z$. Let $p_1(z) = \prod_{j=1}^{m} (z - \xi_j)$ and assuming that all zeros ξ_j of $p_1(z)$ are different[5], then

$$\frac{1}{p_1(z)} = \frac{1}{2\pi i} \int_{C(z)} \frac{1}{\prod_{j=1}^{m} (w - \xi_j)(w-z)} dw$$

Since $\lim_{z \to \infty} \frac{1}{|p_1(z)|} = 0$, we can deform the contour $C(z)$ to enclose the entire complex plane except for an arbitrary small region around the point $w = z$. The function $\frac{1}{p_1(z)}$ is analytic everywhere, except for the simple zeros at $w = \xi_j$. Cauchy's residue theorem (Titchmarsh, 1964) then leads to

$$\frac{1}{p_1(z)} = -\sum_{l=1}^{m} \lim_{w \to \xi_l} \frac{w - \xi_l}{\prod_{j=1}^{m} (w - \xi_j)(w-z)}$$

$$= \sum_{l=1}^{m} \frac{1}{\prod_{j=1;j \neq l}^{m} (\xi_l - \xi_j)} \frac{1}{z - \xi_l} = -\sum_{l=1}^{m} \frac{1}{\prod_{j=1;j \neq l}^{m} (\xi_l - \xi_j)} \sum_{k=0}^{\infty} \frac{z^k}{\xi_l^{k+1}}$$

Thus, we find the Taylor expansion, for $|z| < \min_{1 \leq l \leq m} \xi_l$,

$$\frac{1}{p_1(z)} = \frac{1}{\prod_{j=1}^{m} (z - \xi_j)} = -\sum_{k=0}^{\infty} \left\{ \sum_{l=1}^{m} \frac{1}{\xi_l^{k+1}} \prod_{j=1;j \neq l}^{m} \frac{1}{\xi_l - \xi_j} \right\} z^k \qquad (9.24)$$

Proceeding similarly as in **art.** 209 by computing the Cauchy product of $p_0(z)$ and $\frac{1}{p_1(z)}$, we arrive at

---

[5] When not all zeros are simple, we need to invoke the k-th derivative of the Cauchy integral,

$$\frac{1}{k!} \frac{d^k f(z)}{dz^k} \qquad \frac{1}{2\pi i} \int_{C(z)} \frac{f(w)}{(w\ \ z)^{k+1}} dw \qquad (9.23)$$

$$\frac{p_0\left(z\right)}{p_1\left(z\right)} = \sum_{k=0}^{n\,m} \left\{ \sum_{l=1}^{m} \frac{1}{\xi_l^{k+1} \prod_{j=1;j\neq l}^{m} \left(\xi_l - \xi_j\right)} \sum_{q=k+1}^{n} a_q \xi_l^q \right\} z^k + \sum_{l=1}^{m} \frac{p_0\left(\xi_l\right)}{\prod_{j=1;j\neq l}^{m} \left(\xi_l - \xi_j\right)} \frac{1}{z - \xi_l}$$

(9.25)

Observe from (9.13) that $\prod_{j=1;j\neq l}^{m} \left(\xi_l - \xi_j\right) = F'_m\left(\xi_l\right)$ and that $p_1\left(z\right) = F_m\left(z\right)$ where $x_k = \xi_k$ such that (9.25), when $m = n$, equals

$$p_0\left(z\right) = \sum_{l=1}^{n} p_0\left(\xi_l\right) \frac{F_n\left(z\right)}{\left(z - \xi_l\right) F'_n\left(\xi_l\right)}$$

which is the Lagrange interpolation polynomial (9.16) corresponding to the set of n points $\{(\xi_l, p_0\left(\xi_l\right))\}_{1\leq l\leq n}$. The first sum in (9.25), which reduces to the $k = 0$ term when $n = m$, vanishes because

$$\sum_{l=1}^{n} \frac{p_0\left(\xi_l\right) - p_0\left(0\right)}{\xi_l F'_n\left(\xi_l\right)} = \sum_{l=1}^{n} \frac{p_0\left(\xi_l\right)}{\xi_l F'_n\left(\xi_l\right)} - p_0\left(0\right) \sum_{l=1}^{n} \frac{1}{\xi_l F'_n\left(\xi_l\right)} = 0$$

which follows from the Taylor expansion (9.24) and the Lagrange polynomial, both evaluated at $z = 0$.

We have implicitly assumed that not all ξ_l are zeros of $p_0\left(z\right)$. If all $\{\xi_l\}_{1\leq l\leq m}$ are simple zeros of $p_0\left(z\right)$, then (9.25), written in terms of the polynomial in (9.13), reduces to the quotient polynomial

$$q_m\left(z\right) = \frac{p_0\left(z\right)}{F_m\left(z\right)} = \sum_{k=0}^{n\,m} \left\{ \sum_{l=1}^{m} \frac{\sum_{q=0}^{n\,k\,1} a_{q+k+1} \xi_l^q}{F'_m\left(\xi_l\right)} \right\} z^k$$

(9.26)

Compared to the quotient polynomial (9.21) for $m = 1$, the coefficients in the general version (9.26) of the quotient polynomial only require m similar polynomial evaluations $\sum_{q=0}^{n\,k\,1} a_{q+k+1} \xi_l^q$ as in (9.21) and m additional $F'_m\left(\xi_l\right)$ computations.

211. *Minimal polynomial.* The minimal polynomial associated to a polynomial $p_n\left(z\right) = a_n \prod_{k=1}^{l} \left(z - z_k\right)^{m_k}$, where m_k denotes the multiplicity of zero z_k, is defined as

$$m_{p_n}\left(z\right) = a_n \prod_{k=1}^{l} \left(z - z_k\right)$$

(9.27)

The minimal polynomial divides $p_n\left(z\right)$ and is the lowest degree polynomial possessing the same zeros of $p_n\left(z\right)$, all with multiplicity 1. If $p_n\left(z\right)$ has only simple zeros, i.e., $m_k = 1$ for all $1 \leq k \leq n$, then $m_{p_n}\left(z\right) = p_n\left(z\right)$.

The minimal polynomial plays an important role in matrix polynomials and the Caley Hamilton theorem (**art. 145**).

9.5 Descartes' rule of signs

212. A famous theorem due to René Descartes is:

Theorem 47 (Descartes' rule of signs) *Let C denote the number of changes of sign in the sequence of real coefficients $a_0, a_1, \ldots, a_n$ of a polynomial $p_n(z) = \sum_{k=0}^{n} a_k x^k$ and let Z denote the number of positive real zeros of $p_n(z)$, then*

$$C - Z = 2k \geq 0$$

where k is a non negative integer.

Before proving Theorem 47, we make the following observation. The product form in (9.1) for a real polynomial with v real and $2k$ complex zeros, such that $n = v + 2k$, can be written as

$$p_n(z) = a_n \prod_{j=1}^{v} (z - x_j) \prod_{j=1}^{k} (z - \operatorname{Re} z_j)^2 + (\operatorname{Im} z_j)^2$$

from which

$$a_0 = p_n(0) = a_n \prod_{j=1}^{v} (-x_j) \prod_{j=1}^{k} (\operatorname{Re} z_j)^2 + (\operatorname{Im} z_j)^2$$

shows that the sign of a_0 does not dependent on the complex zeros. For example, a_0 has the sign of a_n if all real zeros x_j are negative. The sequence $a_0, a_1, \ldots, a_n$ in which $\operatorname{sign}(a_0) = \operatorname{sign}(a_n)$, equivalent to $a_0 a_n > 0$, has an even number of changes in sign. This is best verified when the sequence is plot as a piece wise linear function through the points (k, a_k) for $0 \leq k \leq n$, similar as for the random walk in **art.** 132. The number of sign changes equals the number of k axis crossings. Zero coefficients do not contribute to a change in sign. For example, the sequence $\{1, 2, 0, 0, -1, 0, 1\}$ has two sign changes.

Generalizing this observation, if the polynomial $p_n(z)$ with real coefficients has an even number of real, positive zeros such that $\operatorname{sign}(a_0) = \operatorname{sign}(a_n)$, the number C of sign changes in $a_0, a_1, \ldots, a_n$ is even, whereas, if $p_n(z)$ has an odd number of real, positive zeros such that $\operatorname{sign}(a_0) = -\operatorname{sign}(a_n)$, the number C of sign changes is odd. This argument demonstrates that $C - Z = 2k$ is even. To show that k is non negative, a deeper argument is needed.

Proof[6] **(by Laguerre):** Let $z = e^x$, then the number of real zeros of the function $p_n(e^x) = \sum_{k=0}^{n} a_k e^{kx}$ is the same as the number of positive zeros of $p_n(x)$, because $x = \log z$ is monotonous increasing for $z > 0$. Laguerre actually proves a more

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[6] In 1828, Gauss proved Descartes' rule, which was published in 1637 in his *Géométrie*. Laguerre studied and extended Descartes' rule in several papers, combined by Hermite *et al.* (1972) in the part on Algebra.

general result by considering the entire function

$$F(x) = \sum_{k=0}^{n} a_k e^{\lambda_k x}$$

where the real numbers obey $\lambda_0 < \lambda_1 < \cdots < \lambda_n$. Clearly, if we choose $\lambda_k = k$, we obtain the result for $p_n(e^x)$. Let C denote the number of changes in sign in the sequence $a_1, a_2, \ldots, a_n$ and let Z denote the number of real zeros of the entire function $F(x)$. Since for $x \to \infty$, the term $a_n e^{\lambda_n x}$ dominates, while for $x \to -\infty$, the term $a_0 e^{\lambda_0 x}$ is dominant; by the argument above, therefore, $C - Z$ is even. The proof that $C - Z \geq 0$ is by induction. If there are no changes of sign ($C = 0$), then there are no zeros ($Z = 0$) and $C \geq Z$. Assume that the Theorem holds for $C - 1$ changes of sign (hypothesis). Suppose that $F(x)$ has $C > 0$ changes of sign and let $\beta + 1$ be an index of change, i.e., $a_\beta a_{\beta+1} < 0$ for $1 \leq \beta < n$. Consider now the related function

$$G(x) = \sum_{k=0}^{n} a_k (\lambda_k - \lambda) e^{\lambda_k x}$$

then, for $\lambda_\beta < \lambda < \lambda_{\beta+1}$, the number of changes of sign in the sequence

$$-a_0 (\lambda - \lambda_0), -a_1 (\lambda - \lambda_1), \ldots, -a_\beta (\lambda - \lambda_\beta), a_{\beta+1} (\lambda_{\beta+1} - \lambda), \ldots, a_n (\lambda_n - \lambda)$$

is precisely $C_G = C - 1$ because now $-a_\beta (\lambda - \lambda_\beta) a_{\beta+1} (\lambda_{\beta+1} - \lambda) > 0$, where all other consecutive products remain unchanged. Further,

$$G(x) = e^{\lambda x} \frac{d}{dx} \left(e^{-\lambda x} F(x) \right)$$

and, since $e^{-\lambda x} > 0$ for all real x, $e^{-\lambda x} F(x)$ and $F(x)$ have the same real zeros. As a consequence of Rolle's Theorem, the derivative $f'(x)$ has no less than $Z - 1$ zeros in the same interval where $f(x)$ has Z zeros. Hence, $G(x)$ has at least $Z_G \geq Z - 1$ zeros. On the other hand, $G(x)$ has at most $Z - 1$ zeros[7]. Thus, $C_G - Z_G = C - 1 - (Z - 1)$ and, by the induction argument ($C - 1 \geq Z - 1$), we arrive at $C_G \geq Z_G$. Introducing $C_G = C - 1$ and $Z_G = Z - 1$, we finally obtain that $C \geq Z$, which completes the induction. $\qquad \square$

Since the set of exponents $\{\lambda_k\}_{1 \leq k \leq n}$ can be real numbers, Laguerre's proof thus extends Descartes' rule of signs to a finite sum of non integer powers of x. For example, $x^3 - x^2 + x^{1/3} + x^{1/7} - 1 - x^{-2} = 0$ has $C = 3$ sign changes, and thus at most $Z \leq 3$ positive (real) zeros.

Since the polynomial $p_n(-x)$ has coefficients $(-1)^k a_k$, Descartes' rule of signs indicates that the number of negative real zeros of $p_n(x)$ is not larger than the number of changes in signs in $p_n(-x)$.

---

[7] If $f(z)$ is an analytic function in the interior of a single closed contour C defined by $|f(z)| = M$, where M is a constant, then the number of zeros of $f(z)$ in this region exceeds the number of zeros of the derivative $f'(z)$ in that same region by unity (Whittaker and Watson, 1996, p. 121).

Descartes' rule of signs is only exact if $C < 2$ because $k \geq 0$; thus, in case there is no ($C = 0$) or only one ($C = 1$) sign variation, which corresponds to no or exactly one positive real zero. The reverse of the $C = 0$ case holds: if all zeros of a real polynomial have negative real part, then all coefficients are positive and there is no change in sign. However, the reverse implication, $\{Z = 1\} \Longrightarrow \{C = 1\}$ does not hold in general as the example $x^3 - x^2 + x - 1 = (x - 1)(x - i)(x + i)$ shows.

Example 1 The polynomial $p_5(x) = 2x^5 - x^4 + x^3 + 11x^2 - x + 2$ has four changes in sign, while $p_5(-x) = -2x^5 - x^4 - x^3 + 11x^2 + x + 2$ only has one change in sign. Hence, while there are in total precisely five zeros, there is at most one negative real zero and at most four real positive. Since complex zeros appear in pairs, there can be either four, two or zero real positive zeros, but precisely one negative zero.

Example 2 Milovanović *et al.* (1994) mention the remarkable inequality, valid for all real x and even integers $n > 0$,

$$q_n(x) = x^n - nx + n - 1 \geq 0$$

with equality only if $x = 1$. Since $q_n(-x)$ has only positive coefficients, $q_n(-x) > 0$. For $x > 0$, there are $C = 2$ changes in sign and Descartes' rule of signs states that there are at most two real zeros. Since $q_n(1) = q_n'(1) = 0$, the polynomial $q_n(x)$ has a double zero at $x = 1$, which is thus the only real zero and this implies $q_n(x) \geq 0$.

213. *Number of sign changes in the sequence of the differences.* Let C be the number of sign changes in the sequence $a_0, a_1, \ldots, a_n$ and assume that these sign changes occur between the elements

$$(a_{k_1}, a_{m_1}), (a_{k_2}, a_{m_2}), \ldots, (a_{k_C}, a_{m_C})$$

where $k_j \leq m_j - 1$ and the equality sign only occurs if there are no zero elements between a_{k_j} and a_{m_j}. We denote $a_{m_0} = a_0$ and $a_{k_{C+1}} = a_n$, which has the same sign as a_{m_C} and $a_{k_{C+1}+1} = 0$. Assume, without loss of generality, that $a_{m_0} > 0$. Then, we have that $\operatorname{sign} a_{k_j} = (-1)^{i-1}$, $\operatorname{sign} a_{m_j} = (-1)^j$ for $1 \leq j \leq C$ and

$$(-1)^{i-1} a_{m_j-1} \geq 0$$

Consider now the sequence of the differences $a_0, a_1 - a_0, a_2 - a_1, \ldots, a_n - a_{n-1}$. We denote the difference by $\Delta a_j = a_j - a_{j-1}$ for $1 \leq j \leq n$ and $\Delta a_0 = a_0$. The sign of the $1 \leq j \leq C$ elements,

$$(-1)^i (a_{m_j} - a_{m_j-1}) = (-1)^i \Delta a_{m_j} > 0$$

is known. Since Δa_{m_j-1} and Δa_{m_j} have opposite sign for $1 \leq j \leq C$, the changes in sign of all differences between them is odd (an odd number of k axis crossings). The last subsequence between Δa_{m_C} and $\Delta a_{n+1} = a_{n+1} - a_{k_{C+1}} = -\operatorname{sign} a_{m_C} = -\operatorname{sign} \Delta a_{m_C}$ also has an odd number of sign changes. Summing the sign changes in all $C + 1$ subintervals equals C plus an odd number of sign changes. Thus, we have proved:

Lemma 12 *If C is the number of sign changes in the sequence $a_0, a_1, \ldots, a_n$, then the number of sign changes in the sequence of the differences $\Delta a_0, \Delta a_1, \ldots, \Delta a_n$, where $\Delta a_j = a_j - a_{j-1}$ for $1 \leq j \leq n$ and $\Delta a_0 = a_0$, equals C plus an odd positive number.*

214. Consider the polynomial

$$q_{n+1}(x) = (x - \xi) p_n(x) = a_n x^{n+1} + \sum_{k=1}^{n} (a_{k-1} - \xi a_k) x^k - \xi a_0$$

$$= \sum_{j=0}^{n+1} (a_{j-1} - \xi a_j) x^j$$

with the convention that $a_{-1} = a_{n+1} = 0$. If $\xi > 0$, the number of sign changes in the coefficients $b_j = a_{j-1} - \xi a_j$ of $q_{n+1}(x)$ equals the number of sign changes in the difference $\Delta (\xi^j a_j) = \xi^j a_j - \xi^{j-1} a_{j-1} = -\xi^{j-1} b_j$. Lemma 12 shows that the number of sign changes in the difference sequence equals that in the polynomial $p_n(z)$ plus an odd positive number. Descartes' rule of signs, Theorem 47, states that $C_{p_n(z)} = Z_{p_n(z)} + 2k$ and, hence,

$$C_{q_{n+1}(z)} = Z_{p_n(z)} + 2k + 2m + 1 = Z_{q_{n+1}(z)} + 2(k+m)$$

Notice that the argument and Lemma 12 provide a second proof of Descartes' rule of signs, Theorem 47, because we have just shown the inductive step: if the rule holds for $p_n(z)$, it also holds for $q_{n+1}(z)$. Descartes' rule of signs definitely holds for $n = 0$ and this completes the second proof.

If $\xi > 0$ and the number of changes in sign in $p_n(x)$ is zero (which implies by Descartes' rule of signs, Theorem 47, that $p_n(x)$ has no positive real zeros), then ξ is the largest real zero of $q_{n+1}(x)$. If $\xi < 0$ and the coefficients of $p_n(x)$ are alternating (equivalent to the fact that $p_n(x)$ does not have negative real zeros (**art. 212**)), then ξ is the smallest real zero of $q_{n+1}(x)$.

215. Laguerre (see Hermite *et al.* (1972)) has elegantly and ingeniously extended Descartes' rule of signs. As in **art. 212**, Laguerre considers, as a generalization of the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$, the entire function

$$F(z) = \sum_{k=0}^{n} a_k z^{\beta_k} = a_n z^{\beta_n} + a_{n-1} z^{\beta_{n-1}} + \ldots + a_0 z^{\beta_0} \tag{9.28}$$

where $\beta_n > \beta_{n-1} > \ldots > \beta_0$ are real numbers.

Theorem 48 (Laguerre) *The number of real zeros Z of the entire function $F(z)$, defined in (9.28), that are larger than a positive number ξ, is at most equal the number C of changes in signs of the sequence*

$$a_n \xi^{\beta_n}, a_n \xi^{\beta_n} + a_{n-1} \xi^{\beta_{n-1}}, \ldots, F(\xi)$$

and $C - Z = 2k \geq 0$.

Proof: We start from the polynomial identity (9.22),

$$\frac{p_n(z)}{z-\xi} = \sum_{k=0}^{n-1} \left(\sum_{j=k+1}^{n} a_j \xi^{j-k-1} \right) z^k + \frac{p_n(\xi)}{z-\xi}$$

Using the expansion $(z-\xi)^{-1} =$ for $z > \xi$ results in

$$\frac{p_n(z)}{z-\xi} = \sum_{k=0}^{n-1} \left(\sum_{j=k+1}^{n} a_j \xi^{j-k-1} \right) z^k + \sum_{k=0}^{\infty} \frac{\xi^k p_n(\xi)}{z^{k+1}}$$

Laguerre's extension of Descartes' rule of signs (**art.** 212) indicates that the number of real zeros Z of $p_n(z)$ that are larger than ξ is at most equal to the number of sign changes of the right hand side. Since $\xi > 0$, all terms $\xi^k p_n(\xi)$ for $k > 0$ have the same sign as $p_n(\xi)$, which implies that the number C of sign changes is equal to the number of sign changes of the coefficients in the first k sum. Each of these coefficients has the same sign as the partial sum $\sum_{j=k+1}^{n} a_j \xi^j$ of $p_n(\xi)$, because $\xi > 0$. This proves the theorem in case $F(z)$ is a polynomial.

At last, we can always reduce $F(z)$ to a polynomial form. If $\beta_0 < 0$ and all exponents β_k are integers, $z^{-\beta_0} F(x)$ is a polynomial and the above argument applies. If $\beta_k \in \mathbb{Q}^+$, then $F(z^w)$ is a polynomial provided w is the least common multiple of the denominators of the set $\{\beta_k\}_{1 \leq k \leq n}$. Finally, since each real number can be approximated arbitrarily close by a rational number, so can $F(z)$ with real exponents approximated arbitrarily close by a polynomial, which demonstrates Theorem 48. $\square$

Theorem 48 is readily modified when we want the number of *positive* zeros smaller than ξ. In that case, we may verify by following the same steps as in the proof above that the Theorem 48 also holds for the number of *positive* zeros smaller than ξ, provided the order of terms (9.28) is written according to increasing exponents, i.e., $\beta_n < \beta_{n-1} < \ldots < \beta_0$. As a corollary, the number of zeros in $[0,1]$ of $F(z)$ is at most equal to the number of sign changes in the sequence

$$a_n, a_n + a_{n-1}, \ldots, F(1)$$

Another application is $F(z) = p_n(z+h)$, which we expand by Taylor's theorem

$$p_n(z+h) = \sum_{j=0}^{n} \frac{p_n^{(j)}(h)}{j!} z^j = p_n(h) + z p_n'(h) + z^2 \frac{p_n''(h)}{2} + \ldots + z^n \frac{p_n^{(n)}(h)}{n!}$$

into a polynomial, written with exponents of z in increasing order. The number of real zeros of $F(z)$ between $[0, \xi]$, and thus the real zeros of $p_n(z)$ between $[h, h+\xi]$, is at most equal to the number of sign changes in the sequence

$$\left\{ p_n(h), p_n(h) + \xi p_n'(h), p_n(h) + z p_n'(h) + z^2 \frac{p_n''(h)}{2}, \ldots, p_n(\xi+h) \right\}$$

and their difference is an even integer (possibly zero).

The whole idea can subsequently be applied to $\frac{p_n(z)}{(z-\xi)^m}$ using **art. 210**. Since the number of sign changes in $\frac{p_n(z)}{(z-\xi)^m}$ is at most equal to that in $\frac{p_n(z)}{(z-\xi)^{m-1}}$ (**art. 214**), but not smaller than the number of real zeros of $p_n(z)$ larger than ξ, we may expect to deduce, by choosing an appropriate m, an exact way to determine the number of such real zeros. In fact, Laguerre succeeded (Hermite *et al.*, 1972, p. 24 25) to propose an exact method, that involves the discriminant (**art. 201**), which is hard to compute. In summary, his method turns out to be less attractive than that of Sturm, discussed in **art. 225**.

216. We present another nice approach due to Laguerre (Hermite *et al.*, 1972, p. 26 41). Consider the polynomial

$$f_n(z) = \sum_{j=1}^m A_j p_n(\xi_j z)$$

where $0 < \xi_m < \xi_{m-1} < \ldots < \xi_1$ and $p_n(z) = \sum_{k=0}^n a_k z^k$. Explicitly,

$$f_n(z) = \sum_{k=0}^n \left(a_k \sum_{j=1}^m A_j \xi_j^k \right) z^k$$

Descartes' rule of signs, Theorem 47, states that the number Z of positive zeros is at least equal to the number C of variation in sign in the sequence

$$\left\{ a_0 \sum_{j=1}^m A_j, a_1 \sum_{j=1}^m A_j \xi_j, \ldots, a_n \sum_{j=1}^m A_j \xi_j^n \right\}$$

That number C is also equal to the number C_1 of sign changes in the sequence $(l < n)$

$$S_1 = \left\{ a_0 \sum_{j=1}^m A_j, a_1 \sum_{j=1}^m A_j \xi_j, \ldots, a_l \sum_{j=1}^m A_j \xi_j^l \right\}$$

plus the number C_2 of changes of sign in the remaining sequence

$$S_2 = \left\{ a_l \sum_{j=1}^m A_j \xi_j^l, a_{l+1} \sum_{j=1}^m A_j \xi_j^{l+1}, \ldots, a_n \sum_{j=1}^m A_j \xi_j^n \right\}$$

$$= \{ a_l \phi(0), a_{l+1} \phi(1), \ldots, a_n \phi(n-l) \}$$

where

$$\phi(x) = \sum_{j=1}^m A_j \xi_j^l \xi_j^x = \sum_{j=1}^m A_j \xi_j^l (e^x)^{\log \xi_j}$$

If we suppose that all $a_k \geq 0$, then the number C_2 of variations in sign in S_2 is at most equal to the number Z_ϕ of positive zeros of $\phi(x)$ (because even if $\phi(k)\phi(k-1) > 0$, there can be an even number of zeros in the interval $(k-1, k)$).

The number Z_ϕ is also equal to the number of real zeros of $\phi(\log z) = 0$, which is greater than 1. Theorem 48 in **art. 215** shows that the number Z_ϕ of real zeros of $\phi(\log z)$ larger than 1 is at most equal to the number C_ϕ of sign changes in the sequence

$$\left\{ A_1 \xi_1^l, A_1 \xi_1^l + A_2 \xi_2^l, \ldots, \phi(0) \right\}$$

Hence, $Z \le C \le C_1 + C_\phi$. Since the above holds for all $0 \le l < n$, the simplest choice is $l = 0$. Thus, we have proved

Theorem 49 (Laguerre) *The number of real roots Z of the equation*

$$\sum_{j=1}^m A_j p_n(\xi_j z) = 0$$

where $0 < \xi_m < \xi_{m\,1} < \ldots < \xi_1$ and $p_n(z) = \sum_{k=0}^n a_k z^k$, is at most equal to the number of variations in sign of the sequence $\left\{ A_1, A_1 + A_2, \ldots, \sum_{j=1}^m A_j \right\}$.

Theorem 49 holds for $f(z) = \lim_{n\to\infty} p_n(z)$ provided the polynomial sum converges. As an application, we consider $f(z) = e^z$. The equation $\sum_{j=0}^m A_j \exp(\xi_j z) = 0$ possesses the same roots as $\sum_{j=0}^m A_j \exp((\xi_j + k) z) = 0$, where k is a finite real number such that the restriction $0 < \xi_m$ can be removed. Let $\xi_j = a + j\Delta t$ and $\xi_m = b > a$, such that $m = \frac{b\,a}{\Delta t}$, then we obtain the Riemann sum,

$$\lim_{\Delta t \to 0} \sum_{j=1}^{\frac{b\,a}{\Delta t}} A_j e^{(a+j\Delta t)z} \Delta t = \int_a^b e^{xz} \psi(z)\, dz$$

where $\psi(z)$ is a completely arbitrary function (continue or discontinue) because the coefficients $A_0, A_1, \ldots, A_m$ are completely arbitrary. The number of changes in sign in the sequence $\left\{ A_1, A_1 + A_2, \ldots, \sum_{j=1}^{m_1} A_j \right\}$ is, in that limit, at most equal to the number of zeros of $\int_a^x \psi(z)\, dz = 0$ in the interval (a, b). For example, let

$$\psi(z) = \sum_{k=0}^n a_k \frac{z^{\beta_k + w\,1}}{\Gamma(\beta_k + w)}$$

where all $\beta_k > 0$, $w \ge 0$ and $\Gamma(x)$ is the Gamma function. For $a = 0$ and $b = \infty$, the equation $\int_0^\infty e^{xz} \psi(z)\, dz = 0$ becomes

$$\sum_{k=0}^n \frac{a_k}{x^{\beta_k + w}} = 0$$

whose number of positive zeros is, after the transformation $x \to x^{\,1}$, precisely equal to those of $\sum_{k=0}^n a_k x^{\beta_k + w} = 0$ and, thus, of $\sum_{k=0}^n a_k x^{\beta_k} = 0$. On the other hand, the number of positive zeros of the equation $\int_0^x \psi(z)\, dz = 0$, computed as

$$\sum_{k=0}^n a_k \frac{x^{\beta_k + w}}{\Gamma(\beta_k + w + 1)} = 0$$

is at least equal to those of $\sum_{k=0}^{n} a_k x^{\beta_k} = 0$. Now, for $\beta_k = k$ the equations reduce to polynomials and we observe that, after a transform $x \to -x$, the number of negative zeros of the polynomial $p_n(x) = \sum_{k=0}^{n} a_k x^k$ is at most equal to those of the polynomial $\sum_{k=0}^{n} a_k \frac{x^k}{\Gamma(k+w+1)}$. Consequently, we arrive at

Theorem 50 (Laguerre) *If all zeros of the polynomial $p_n(x) = \sum_{k=0}^{n} a_k x^k$ are real, then the zeros of the related polynomial $q_n(x; w) = \sum_{k=0}^{n} a_k \frac{x^k}{\Gamma(k+w+1)}$ are also all real, for any real number $w \geq 0$.*

Many extensions of Laguerre's Theorem 50 have been deduced, the so called *zero mapping transformations*. Consider the set of real numbers $\{\gamma_k\}_{k\geq 0}$, which is a zero mapping transformation, satisfying certain properties. If all zeros of the polynomial $p_n(x) = \sum_{k=0}^{n} a_k x^k$ are real, then the zeros of the related, transformed polynomial $t_n(x; \gamma) = \sum_{k=0}^{n} \gamma_k a_k x^k$ are also all real. A large list of particular sequences $\{\gamma_k\}_{k\geq 0}$ is presented in Milovanović *et al.* (1994).

217. Theorem 50 in **art.** 216 can be extended,

Theorem 51 (Laguerre) *Let $p_n(z) = \sum_{k=0}^{n} a_k z^k$ be a polynomial with real zeros and let $f(z)$ be an entire function (of genus 0 or 1), which is real for real z and all the zeros are real and negative. Then, the polynomial*

$$g_n(z) = \sum_{k=0}^{n} a_k f(k) z^k$$

has all real zeros, and as many positive, zero and negative zeros as $p_n(z)$.

Proof: See Hermite *et al.* (1972, p. 200) or Titchmarsh (1964, pp. 268 269). □

It can be shown (Titchmarsh, 1964, pp. 269 270) that, if $n \to \infty$ and $p(z) = \lim_{n\to\infty} p_n(z)$ is an entire function, then $g(z) = \lim_{n\to\infty} g_n(z)$ is entire, all of whose zeros are real and negative. Hence, applied to $p(z) = e^z$, Laguerre's theorem (extended to $n \to \infty$) shows that the Taylor series

$$g(z) = \sum_{k=0}^{\infty} \frac{f(k)}{k!} z^k$$

is an entire function $g(z)$ with negative, real zeros.

218. The polynomial

$$r_n(z) = |a_n| z^n - \sum_{k=0}^{n-1} |a_k| z^k$$

where $|a_n| > 0$ and $\sum_{k=0}^{n-1} |a_k| > 0$, has precisely one positive zero. Descartes' rule of signs, Theorem 47, tells us that there is at most one positive zero because there

is one change of sign. We show that there is precisely one zero by noting that in

$$r_n(z) = |a_n| z^n \left(1 - \sum_{k=0}^{n-1} \frac{|a_k|}{|a_n|} z^{k-n}\right)$$

the k sum is monotone decreasing from ∞ to 0 when z increases from 0 to ∞. Hence, there is precisely one point $z = \zeta$ at which the k sum is 1 and $r_n(\zeta) = 0$. Moreover, $r_n(z) < 0$ if $z < \zeta$ and $r_n(z) > 0$ if $z > \zeta$.

Consider now

$$\tilde{r}_n(z) = z^n r_n(z^{-1}) = |a_n| - \sum_{k=1}^{n} |a_{n-k}| z^k$$

The same argument as above for the k sum demonstrates that there is precisely one positive zero, which is by **art. 196**, equal to ζ^{-1}.

219. *If z_0 is a zero of $p_n(z) = a_n z^n + \sum_{k=0}^{n-1} a_k z^k$ and ζ is the only positive zero of $r_n(z) = |a_n| z^n - \sum_{k=0}^{n-1} |a_k| z^k$ in **art. 218**, then $|z_0| \le \zeta$.*

Proof:

$$|a_n| |z_0^n| = \left| -\sum_{k=0}^{n-1} a_k z_0^k \right| \le \sum_{k=0}^{n-1} |a_k| |z_0|^k = |a_n| |z_0|^n - r_n(|z_0|)$$

which shows that $0 \le -r_n(|z_0|)$. **Art.** 218 indicates that this condition, equivalent to $r_n(|z_0|) \le 0$, implies that $|z_0| \le \zeta$. □

Similarly, the absolute values of the zeros of $p_n(z)$ are larger than or equal to the only positive zero of $\tilde{r}_n(z) = |a_n| - \sum_{k=1}^{n} |a_{n-k}| z^k$.

220. *Cauchy's rule.* We derive an upperbound $\zeta \ge 0$ for any positive zero of the real polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$, without resorting to Decartes' rule. The upperbound $\zeta \ge 0$ satisfies

$$0 \le \left| \frac{p_n(\zeta)}{a_n} \right| = \left| \zeta^n + \sum_{k=0}^{n} \frac{a_k}{a_n} \zeta^k \right| \le \zeta^n + \sum_{k=0}^{n} \left| \frac{a_k}{a_n} \right| \zeta^k$$

Since the coefficients of $p_n(z)$ are real, we rewrite the latter bound as

$$\zeta^n \left(1 - \sum_{k=0 \text{ and } \frac{a_k}{a_n} < 0}^{n-1} \frac{a_k}{a_n} \zeta^{k-n}\right) + \sum_{k=0 \text{ and } \frac{a_k}{a_n} \ge 0}^{n-1} \frac{a_k}{a_n} \zeta^k \ge 0$$

Let us denote $c_k = \left| \frac{a_k}{a_n} \right| \zeta^{k-n}$ for all k indices for which $\frac{a_k}{a_n} < 0$. Then, $\zeta = \left(\frac{|a_k|}{c_k |a_n|} \right)^{1/(n-k)}$ and the above inequality requires that

$$\sum_{k=0 \text{ and } \frac{a_k}{a_n} < 0}^{n-1} c_k \le 1 \tag{9.29}$$

Since all $c_k \geq 0$, we observe that any zero of $p_n(z)$ is not larger than

$$\zeta = \max_{0 \leq k \leq n-1 \text{ and } \frac{a_k}{a_n} < 0} \left(\left(\frac{|a_k|}{c_k |a_n|} \right)^{1/(n-k)} \right) \leq \max_{0 \leq k \leq n-1} \left(\left(\frac{|a_k|}{c_k |a_n|} \right)^{1/(n-k)} \right)$$

$$(9.30)$$

which is Cauchy's rule. If μ denotes the number of negative coefficients of $\frac{p_n(z)}{a_n}$, then $\sum_{k=0 \text{ and } \frac{a_k}{a_n} < 0}^{n-1} 1 \leq \mu$ and the choice $c_k = \frac{1}{\mu}$ clearly satisfies the condition (9.29), leading to

$$\zeta = \max_{0 \leq k < n \text{ and } \frac{a_k}{a_n} < 0} \left(\mu \left| \frac{a_k}{a_n} \right| \right)^{\frac{1}{n-k}}$$

$$(9.31)$$

A weaker bound, derived from the inequality in (9.30), follows from the choice $c_k = \frac{1}{n} \leq \frac{1}{\mu}$. Another choice, that satisfies (9.29) for all k, is $c_k = \frac{\binom{n-1}{k}}{2^{n-1}}$.

221. The equation $p_n(z) = 0$ where $a_n \neq 0$ can be transformed by the substitution $z = bx$ into

$$x^n + \sum_{k=0}^{n-1} \frac{a_k}{a_n} b^{k-n} x^k = 0$$

Let us confine to odd n. Odd polynomials with real coefficients have at least one real zero. We now choose b such that $\frac{a_0}{a_n} b^{-n} = -1$ or $b = \left(-\frac{a_0}{a_n} \right)^{1/n}$. This choice reduces the original equation into

$$q_n(x) = x^n - \sum_{k=1}^{n-1} \frac{a_k}{a_0} \left(-\frac{a_0}{a_n} \right)^{k/n} x^k - 1 = 0$$

Since $q_n(0) = -1 < 0$ and $\lim_{x \to \infty} q_n(x) > 0$, there must lie at least one real root in the interval $(0, \infty)$. If $q_n(1) > 0$, the root must lie between 0 and 1; if $q_n(1) < 0$, then the root lies in the interval $(1, \infty)$. By the transform $x = y^{-1}$, the interval $(1, \infty)$ can be changed to $(0, 1)$. Alternatively, **art. 196** shows that $\prod_{k=1}^{n} z_k = 1$ which indicates that not all zeros can lie in $(0, 1)$ nor in $(1, \infty)$. Hence, we have reduced the problem to find a real zero of $p_n(z)$ with n odd, into a new problem of finding the real root of $q_n(x)$ in $(0, 1)$. We refer to Lanczos (1988) for a scheme of successively lowering the order of the polynomial $q_n(x)$ by shifted Chebyshev polynomials.

222. *Isolation of real zeros via continued fractions.* Let $m_1 \in \mathbb{N}$ and $m_k \in \mathbb{N}_0$ for all $k > 1$.

Theorem 52 (Vincent-Uspensky-Akritas) *There exists a continued fraction transform with a non negative m_1 and further positive integer partial quotients* $\{m_k\}_{2 \leq k \leq l}$,

$$z = \frac{A_l w + A_{l-1}}{B_l w + B_{l-1}} = m_1 + \cfrac{1}{m_2 + \cdots + \cfrac{1}{m_l + w}}$$

$$(9.32)$$

that transforms the polynomial $p_n(z)$ with rational *coefficients a_k and simple zeros into the function $p_n\left(\frac{A_l w + A_{l-1}}{B_l w + B_{l-1}}\right) = (B_l w + B_{l-1})^{-n} \tilde{p}_n(w)$ such that the polynomial $\tilde{p}_n(w)$ has either zero or one sign variation. The integer l is the smallest integer such that $F_{l-1}\frac{d}{2} > 1$ and $F_l{}_{-1}F_l d > 1 + \varepsilon_n{}^{-1}$, where d is the minimum distance between any two zeros, F_m is the m th Fibonacci number that obeys $F_m = F_{m-1} + F_{m-2}$ for $m > 1$ and with $F_0 = F_1 = 1$ and where $\varepsilon_n = \left(1 + \frac{1}{n}\right)^{\frac{1}{n-1}} - 1$.*

Proof: See Akritas (1989, p. 367–371). □

While the converse of Descartes' Theorem 47 in case $C = 0$, implying that there is no positive real zero, is generally true, the converse of the case $C = 1$ is not generally true as demonstrated in **art.** 212. The part of Theorem 52 that details the determination of the integer l guarantees that, if there is one zero with positive real part and all others have negative real part and lying in an ε_n disk around -1, the corresponding polynomial has exactly one change in sign. The Fibonacci numbers F_m enter the scene because they are the denominators of the m th convergent of the continued fraction of the golden mean (see e.g. Govers *et al.* (2008, p. 316)),

$$\frac{1 + \sqrt{5}}{2} = 1 + \cfrac{1}{1 + \cdots + \cfrac{1}{1 + \cfrac{1}{1 + \ddots}}}$$

in the limit case where all $m_k = 1$ for $k \geq 1$. The continued fraction transform (9.32) roughly maps one zero to the interval $(0, \infty)$ and all others in clusters around -1 with negative real part. Moreover, it is equivalent to a series of successive substitutions of the form $z = m_j + \frac{1}{w}$ for $1 \leq j \leq l$. The best way to choose the set of integers $\{m_k\}_{1 \leq k \leq l}$ is still an open issue. Akritas (1989) motivates to choose m_j in each substitution round equal to Cauchy's estimate (9.31). Finally, Akritas (1989) claims that his method for isolating a zero is superior in computational effort to Sturm's classical bisection method based on Theorem 54.

9.6 The number of real zeros in an interval

223. *The Cauchy index.* Consider the rational function $r(z) = \frac{p_m(z)}{p_n(z)}$ that has at most n poles, the zeros of the polynomial $p_n(z)$ that are not zeros of the numerator polynomial $p_m(z)$. We further assume $n > m$, else we can always reduce the rational function as the sum of a polynomial and a rational function, where the numerator polynomial has a smaller degree than the denominator polynomial as explained in **art.** 208. If ζ_k is a zero with multiplicity m_k of $p_n(z)$ but not of $p_m(z)$, then

$$r(z) = p_j(z) \prod_{k=1}^{l} (z - \zeta_k)^{-m_k}$$

where $p_j(z)$ is a polynomial of degree $j \leq m$ and $p_j(\zeta_k) \neq 0$. The behavior of

$r(z)$ around a pole ζ_q of order m_q is dominated by $b_q (z - \zeta_q)^{m_q}$, where $b_q = p_j (\zeta_q) \prod_{k=1; k\neq q}^{l} (\zeta_q - \zeta_k)^{m_k} \neq 0$.

The Cauchy index of a rational function $r(z)$ at a *real* pole y is defined to be $+1$ if

$$\lim_{x\to y} r(x) = -\infty \quad \text{and} \quad \lim_{x\to y^+} r(x) = \infty$$

and the Cauchy index is -1 if

$$\lim_{x\to y} r(x) = \infty \quad \text{and} \quad \lim_{x\to y^+} r(x) = -\infty$$

while the Cauchy index is zero if both limits are the same. Hence, the Cauchy index at ζ_q (assumed to be real) equals 0 if m_q is even and $\text{sign}(b_q)$ if m_q is odd. The Cauchy index of a rational function r for the interval $[a, b]$, denoted by $I_a^b r(x)$ is defined as the sum of the Cauchy indices at all real poles y between a and b, such that $a < y < b$ and a and b are not poles of r.

Now, let $p_n(z) = \prod_{k=1}^{l} (z - \zeta_k)^{m_k}$ and consider its logarithmic derivative

$$r(z) = \frac{d \log p_n(z)}{dz} = \frac{p_n'(z)}{p_n(z)} = \sum_{k=1}^{l} \frac{m_k}{z - \zeta_k} = \sum_{k=1}^{s} \frac{m_k}{z - \zeta_k} + r_1(z)$$

where only the first s zeros are real in the interval $[a, b]$. The Cauchy index of r for the interval $[a, b]$, $I_a^b \frac{p_n'(x)}{p_n(x)} = s$. Hence, $I_a^b \frac{p_n'(x)}{p_n(x)}$ is equal to the number of distinct real zeros of $p_n(z)$ in the interval $[a, b]$. Since $p_n(z)$ has a finite number of zeros, $I_{\infty}^{+\infty} \frac{p_n'(x)}{p_n(x)}$ equals all distinct real zeros of $p_n(z)$. The remainder of the subject thus consists in finding the Cauchy index for the logarithmic derivative in order to determine the number of real zeros of a polynomial in a (possibly infinite) interval $[a, b]$. One of the methods is based on Sturm's classical theorem.

224. *A Sturm sequence.* A sequence of real polynomials $f_1(x), f_2(x), \ldots, f_m(x)$ is a Sturm sequence on the interval (a, b) if it obeys two properties: (i) $f_m(x) \neq 0$ for $a < x < b$ and (ii) $f_{k-1}(x) f_{k+1}(x) < 0$ for any k where $f_k(x) = 0$ and $a < x < b$.

Let $V(x)$ denote the number of changes in sign of the sequence $f_1(x), f_2(x), \ldots, f_m(x)$ at a fixed $x \in (a, b)$. It is clear that the value of $V(x)$ can only change when x varies from a to b, if one of the functions $f_k(x)$ passes through zero. However, for a Sturm sequence, property (ii) shows that, when $f_k(x) = 0$ for any $2 \leq k \leq m-1$, the value of $V(x)$ does not change. Only if $f_1(x)$ passes through a zero $\xi \in (a, b)$, $V(x)$ changes by ± 1 according to the Cauchy index of $\frac{f_2(x)}{f_1(x)}$ at $x = \xi$. Hence, we have shown:

Theorem 53 (Sturm) *If $f_1(x), f_2(x), \ldots, f_m(x)$ is a Sturm sequence on the interval (a, b), then*

$$I_a^b \frac{f_2(x)}{f_1(x)} = V(a) - V(b)$$

225. An interesting application of a Sturm sequence is its connection to the Euclid
ean algorithm (**art.** 208), which we modify (all remainders have negative sign) into

$$p_0(z) = q_1(z)\,p_1(z) - p_2(z) \qquad\qquad (0 < \deg p_2 < \deg p_1)$$
$$p_1(z) = q_2(z)\,p_2(z) - p_3(z) \qquad\qquad (0 < \deg p_3 < \deg p_2)$$
$$p_2(z) = q_3(z)\,p_3(z) - p_4(z) \qquad\qquad (0 < \deg p_4 < \deg p_3)$$
$$\cdots \qquad\qquad\qquad\qquad \cdots$$
$$p_{m\,2}(z) = q_{m\,1}(z)\,p_{m\,1}(z) - p_m(z) \quad (0 < \deg p_m < \deg p_{m\,1})$$
$$p_{m\,1}(z) = q_m(z)\,p_m(z)$$

The sequence $\{p_k(x)\}_{0 \le k \le m}$ is a Sturm sequence if the largest common divisor
polynomial $p_m(x)$ does not change sign in the interval (a, b). By the modified
Euclidean construction, we observe that property (ii) in **art.** 224 is always fulfilled.
Indeed, in the modified Euclidean algorithm for any $0 \le k < m$ and $x \in (a, b)$
relation $p_{k\,1}(x) = q_k(x)\,p_k(x) - p_{k+1}(x)$ shows that, if $p_k(x) = 0$, both $p_{k\,1}(x)$
and $p_{k+1}(x)$ have opposite sign and do not contribute to changes in $V(x)$.

The Euclidean algorithm, applied to the logarithmic derivative $r(z) = \frac{p'(z)}{p(z)}$
where $p_0(z) = p(x)$ and $p_1(z) = p'(z)$, provides information about the multiplicity
of zeros of the polynomial $p(z)$. If ξ is a zero with multiplicity m of $p(z)$, then it is
a zero with multiplicity $m-1$ of $p'(z)$. Hence, both $p(z)$ and $p'(z)$ have the factor
$(z - \xi)^{m\,1}$ in common, and since, by construction, $p_m(z)$ is the largest common
divisor polynomial, $p_m(z)$ also must possess the factor $(z - \xi)^{m\,1}$.

In summary, applying the (modified) Euclidean algorithm to the logarithmic
derivative $r(x) = \frac{p'(x)}{p(x)}$ of a polynomial $p(x)$, **art.** 223 with Theorem 53 leads to:

Theorem 54 (Sturm) *Let $p(z)$ be a polynomial with real coefficients and let
$\{p_k\}$ be the sequence of polynomials generated by the (modified) Euclidean algorithm
starting with $p_0(z) = p(z)$ and $p_1(z) = p'(z)$. The polynomial $p(z)$ has exactly
$V(a) - V(b)$ distinct real zeros in (a, b), where $V(x)$ denotes the number of changes
of sign in the sequence $\{p_k(x)\}$. A complex number ξ is a zero of multiplicity m
of $p(z)$ if and only if ξ is a zero of multiplicity $m - 1$ of $p_m(z)$. Thus, all zeros of
$p(z)$ in (a, b) are simple if and only if $p_m(z)$ has no zeros in (a, b).*

Example Let $p(z) = z^4 - 2z^2 + z + 1$. Descartes' rule of signs (Theorem 47)
states that there are either 2 or 0 real positive zeros. The (modified) Euclidean
algorithm yields, with $p_0(z) = p(z)$ and $p_1(z) = p'_0(z)$,

$$p_0(z) = z^4 - 2z^2 + z + 1 = \left(\frac{z}{4}\right) p_1(z) - \left(z^2 - \frac{3}{4}z - 1\right)$$

$$p_1(z) = 4z^3 - 4z + 1 = (4z + 3)\,p_2(z) - \left(-\frac{9}{4}z - 4\right)$$

$$p_2(z) = z^2 - \frac{3}{4}z - 1 = \left(-\frac{4z}{9} + \frac{91}{81}\right) p_3(z) - \frac{283}{81}$$

and

$$p_3(z) = -\frac{9}{4}z - 4 = \left(\frac{729}{1132}z + \frac{324}{283}\right)p_4(z)$$

$$p_4(4) = -\frac{283}{81}$$

The corresponding continued fraction of the modified Euclidean algorithm is

$$\frac{p_0(z)}{p_1(z)} = q_1(z) - \cfrac{1}{q_2(z) - \cfrac{1}{q_3(z) - \cfrac{1}{\ddots \cfrac{1}{q_m(z)}}}}$$

and, here,

$$\frac{p_0(z)}{p_1(z)} = \frac{z}{4} - \cfrac{1}{4z + 3 - \cfrac{1}{\frac{4z}{9} + \frac{91}{81} - \cfrac{1}{\frac{729}{1132}z + \frac{324}{283}}}}$$

The sequence of signs at $z = 0$ is $+, +, -, -, -$ such that $V(0) = 1$. For $z \to \infty$, the sign of the leading coefficients are $+, +, +, -, -$ and $V(\infty) = 1$, while $V(-\infty) = 3$. There is no positive real zero, but two negative zeros ones. The zeros are simple because $p_4(z)$ is constant. The zeros of $p(z)$ are $z_1 = -1.49$, $z_2 = -0.52$, $z_{3,4} = 1.01 \pm 0.51i$.

9.7 Locations of zeros in the complex plane

226. Consider the real numbers[8] $m_1 > 0$, $m_2 > 0,\dots$, $m_n > 0$ and $\sum_{j=1}^{n} m_j = 1$, and let $\{z_k\}_{1 \le k \le n}$ denote the n complex zeros of a polynomial $p_n(z)$, then the center of gravity is defined as

$$z = \sum_{j=1}^{n} m_j z_j \tag{9.33}$$

and the number m_j can be interpreted as a mass placed at the position z_j. If we consider all possible sets $\{m_j\}_{1 \le j \le n}$ of masses at the fixed points $\{z_k\}_{1 \le k \le n}$ in the complex plane, then the corresponding centers of gravity cover the interior of a convex polygon, the smallest one containing the points $z_1, z_2, \dots, z_n$. The only exception occurs if all zeros lie on a straight line. In that case, all the centers of gravity lie in the smallest line segment that contains all the points $z_1, z_2, \dots, z_n$.

Any straight line through the center of gravity[9] separates the set $\{z_k\}_{1 \le k \le n}$ into

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[8] Here m_k is not the multiplicity of zero z_k.
[9] We may also interpret the vector z_j — z as a force directed from z to z_j with magnitude $m_j|z_j$ — $z|$. Then z represents an equilibrium position of a material point subject to repellant forces exerted by the points $z_1, z_2, \dots, z_n$. If z were outside the smallest convex polygon that contains the z_j's, the resultant of the the several forces acting on z could not vanish: no equilibrium were possible.

parts, one of each side of the line (except if all the points $z_1, z_2, \ldots, z_n$ lie on a line). Indeed, since $\sum_{j=1}^{n} m_j = 1$, we can write (9.33)

$$0 = \sum_{j=1}^{n} m_j (z_j - z)$$

If all the points $w_1, w_2, \ldots, w_n$ are on the same side of a straight line passing through the origin, then $\sum_{j=1}^{n} w_j \neq 0$ and $\sum_{j=1}^{n} \frac{1}{w_j} \neq 0$. Indeed, we can always rotate the coordinate axis such that the imaginary axis coincides with the straight line through the origin. If all points are on one side, then they lie in either the positive or negative half plane and $\sum_{j=1}^{n} \operatorname{Re}(w_j) = \operatorname{Re}\left(\sum_{j=1}^{n} w_j\right)$ and $\sum_{j=1}^{n} \operatorname{Re}\left(w_j^{-1}\right)$ is non zero. Now, let $m_j (z_j - z) = w_j$ and the above argument shows that not all the points $m_j (z_j - z)$ lie on the same side of a line. Translate the origin from the center of gravity z to any other point in the plane and verify that the property still holds.

Theorem 55 (Gauss) *All zeros of the derivative $p'_n(z)$ of a polynomial $p_n(z)$ do not lie outside the smallest convex polygon that contains all the zeros of $p_n(z)$.*

Proof: Let $z_1, z_2, \ldots, z_n$ denote the zeros of $p_n(z)$ and let w be a zero of $p'_n(z)$, different from $z_1, z_2, \ldots, z_n$, then

$$\frac{p'_n(w)}{p_n(w)} = \sum_{j=1}^{n} \frac{1}{w - z_j} = 0$$

or, since also the complex conjugate $\sum_{j=1}^{n} \frac{1}{(w - z_j)^*} = 0$, we have that

$$\sum_{j=1}^{n} \frac{w - z_j}{|w - z_j|^2} = 0$$

This is equivalent to $w \sum_{j=1}^{n} \frac{1}{|w - z_j|^2} = \sum_{j=1}^{n} \frac{1}{|w - z_j|^2} z_j$. With $M = \sum_{j=1}^{n} \frac{1}{|w - z_j|^2}$, we arrive at

$$w = \sum_{j=1}^{n} \frac{1}{M |w - z_j|^2} z_j$$

which expresses a center of gravity if $m_j = \frac{1}{M |w - z_j|^2}$ in (9.33) and, by construction, $\sum_{j=1}^{n} m_j = 1$. Above it is shown that any center of gravity lies inside the smallest convex polygon formed by the points $z_1, z_2, \ldots, z_n$. $\square$

Any smallest convex polygon containing all zeros can be enclosed by a circular disk C because all zeros are finite. If c is a point lying on the boundary of the circle C, then the Möbius transform $s = t(z) = \frac{1}{z - c}$ maps the disk into a half plane (containing the point at infinity, since $s(c) = \infty$). Further considerations of Gauss's Theorem 55 and the Möbius transform are discussed in Henrici (1974).

227. There exists a quite remarkable result that relates the zeros of two polyno mials, that satisfy the *apolar* condition. Two polynomials $p_n(z) = \sum_{k=0}^{n} a_k z^k$ and $q_n(z) = \sum_{k=0}^{n} b_k z^k$ are called *apolar* if they satisfy

$$\sum_{k=0}^{n} (-1)^k \frac{a_k b_{n\ k}}{\binom{n}{k}} = 0 \tag{9.34}$$

Let $\beta_k = \frac{(\ 1)^k b_k}{\binom{n}{k}}$, then the Cauchy product of the polynomials $p_n(z)$ and $\tilde{q}_n(z) = \sum_{k=0}^{n} \beta_k z^k$ is

$$p_n(z)\,\tilde{q}_n(z) = \sum_{k=0}^{2n} \left(\sum_{j=0}^{k} a_j \beta_{k\ j} \right) z^k$$

which shows that the apolar condition (9.34) implies that the n th coefficient or n th derivative at $z = 0$ of the product $p_n(z)\,\tilde{q}_n(z)$ is zero.

Theorem 56 (Grace) *Let $p_n(z) = \sum_{k=0}^{n} a_k z^k$ and $q_n(z) = \sum_{k=0}^{n} b_k z^k$ be apolar, thus satisfying (9.34). Suppose that all zeros of $p_n(z)$ lie in a circular region R, then $q_n(z)$ has at least one zero in R.*

Proof: See, e.g., Szegő (1922), Henrici (1974, pp. 469 472). □

Example Consider $q_n(z) = z^n + b_{n\ k} z^{n\ k}$, whose coefficient $b_{n\ k}$ is chosen to satisfy the apolar condition (9.34), such that $a_0 + (-1)^k \binom{n}{k}^{-1} a_k b_{n\ k} = 0$. Thus, for $b_{n\ k} = (-1)^{k+1} \binom{n}{k} \frac{a_0}{a_k}$, the zeros of $q_n(z)$ are $[0]^{n\ k}$ and $(b_{n\ k})^{1/k} e^{2\pi l/k}$ for $0 \le l < k$. All zeros of $q_n(z)$ lie at the origin or on the circle R around the origin with radius $\left| \binom{n}{k} \frac{a_0}{a_k} \right|^{1/k}$. Grace's Theorem 56 states that, there is at least one zero of $p_n(z)$ that lies inside that circle R.

The example shows that, by choosing an appropriate polynomial $q_n(z)$ whose zeros are known and that can be made apolar to $p_n(z)$, valuable information about the locations of some zeros of $p_n(z)$ can be derived.

Related to Grace's Theorem 56 is:

Theorem 57 (Szegő's Composition Theorem) *Suppose that all the zeros of $p_n(z) = \sum_{k=0}^{n} a_k \binom{n}{k} z^k$ lie in a circular region R. If η is a zero of $q_n(z) = \sum_{k=0}^{n} b_k \binom{n}{k} z^k$, then each zero ξ of $w_n(z) = \sum_{k=0}^{n} a_k b_k \binom{n}{k} z^k$ can be written as $\xi = -s\eta$, where s is a point belonging to R.*

Proof: See Szegő (1922). □

228. Let us assume that there is no zero of the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ in a disk around z_0 with radius ρ. After transforming $z \to z - z_0$, we obtain the polynomial expansion around z_0, $p_n(z) = \sum_{k=0}^{n} b_k(z_0)(z - z_0)^k$, where $b_0(z_0) =$

$p_n(z_0) \neq 0$, by the assumption. Further, we bound $p_n(z)$ for $|z - z_0| < \rho$ as

$$|p_n(z)| = \left| b_0(z_0) + \sum_{k=1}^{n} b_k(z_0)(z - z_0)^k \right| > |b_0(z_0)| - \sum_{k=1}^{n} |b_k(z_0)|(z - z_0)^k$$

$$> |b_0(z_0)| - \sum_{k=1}^{n} |b_k(z_0)| \rho^k = |b_0(z_0)| \left\{ 1 - \sum_{k=1}^{n} \frac{|b_k(z_0)|}{|b_0(z_0)|} \rho^k \right\}$$

Cauchy's rule in **art. 220** shows that we may deduce a sharper bound if all coefficients $b_k(z_0)$ are real. There is exactly one positive solution for ρ of $|b_0(z_0)| = \sum_{k=1}^{n} |b_k(z_0)| \rho^k$ because the right hand side is monotonously increasing from zero (at $\rho = 0$) on. Since finding such solution is, generally not easy, we proceed as in **art. 220**. Let $\beta_k = \frac{|b_k(z_0)|}{|b_0(z_0)|} \rho^k > 0$, for each k where $|b_k(z_0)| > 0$, then

$$|p_n(z)| > |b_0(z_0)| \left\{ 1 - \sum_{k=1; |b_k(z_0)|>0}^{n} \beta_k \right\} \geq |b_0(z_0)| \left\{ 1 - \sum_{k=1}^{n} \beta_k \right\}$$

It suffices to require that $\sum_{k=1}^{n} \beta_k \leq 1$ to obtain $|p_n(z)| > 0$. Hence, given a set of positive numbers β_k satisfying $\sum_{k=1}^{n} \beta_k \leq 1$, then there are no zeros in a disk around z_0 with radius

$$\rho = \min_{1 \leq k \leq n; |b_k(z_0)|>0} \beta_k^{1/k} \left| \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k}$$

Example 1 If $\beta_k = 2^{-k}$ for which $\sum_{k=1}^{n} \beta_k = \sum_{k=1}^{n} 2^{-k} < \sum_{k=1}^{\infty} 2^{-k} = 1$, then a zero free disk around z_0 has radius

$$\rho = \frac{1}{2} \min_{1 \leq k \leq n; |b_k(z_0)|>0} \left| \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k}$$

Example 2 If $\beta_k = \binom{n}{k} y^k (1-y)^{n-k}$, then $\sum_{k=1}^{n} \beta_k = \sum_{k=1}^{n} \binom{n}{k} y^k (1-y)^{n-k} = 1$ and

$$\rho = \frac{y}{1-y} \min_{1 \leq k \leq n; |b_k(z_0)|>0} (1-y)^{\frac{n}{k}} \left| \binom{n}{k} \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k}$$

If $0 < y < 1$, then $(1-y)^{\frac{n}{k}} < (1-y)^n$ such that

$$\rho \geq y(1-y)^{n-1} \min_{1 \leq k \leq n; |b_k(z_0)|>0} \left| \binom{n}{k} \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k}$$

Finally, the maximum of $y(1-y)^{n-1}$ occurs at $y = \frac{1}{n}$ and is $\frac{1}{n}\left(1 - \frac{1}{n}\right)^{n-1} > \frac{1}{ne}$. Thus, a zero free disk around z_0 has radius

$$\rho = \frac{1}{ne} \min_{1 \leq k \leq n; |b_k(z_0)|>0} \left| \binom{n}{k} \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k}$$

Example 2 has another interesting property: Vieta's formulae (9.9) applied to $p_n(z) = \sum_{k=0}^{n} b_k(z_0)(z - z_0)^k$ shows that

$$\frac{b_m(z_0)}{b_0(z_0)} = (-1)^m \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_m=j_{m-1}+1}^{n} \prod_{i=1}^{m} \frac{1}{z_{j_i} - z_0}$$

where the multiple sum contains $\binom{n}{m}$ terms as shown in **art. 199**. Now, let $d = \min_{1 \le k \le n} |z_k - z_0|$ denote the distance of the z_0 to the nearest zero of $p_n(z)$, then $|z_k - z_0|^{-1} \le d^{-1}$ for all $1 \le k \le n$. Introduced in the above Vieta formula yields, for $1 \le m \le n$,

$$\left| \frac{b_m(z_0)}{b_0(z_0)} \right| = \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_m=j_{m-1}+1}^{n} \prod_{i=1}^{m} \left| \frac{1}{z_{j_i} - z_0} \right| \le \binom{n}{m} d^{-m}$$

from which

$$d \le \min_{1 \le k \le n; |b_k(z_0)|>0} \left| \binom{n}{k} \frac{b_k(z_0)}{b_0(z_0)} \right|^{1/k} = ne\rho$$

Thus, we have shown that there is at least one zero in the disk around z_0 with radius $ne\rho$, while Example 2 demonstrates that there are no zeros in the disk with the same center z_0 but radius ρ. Finally, we use the bound $\left| \frac{b_m(z_0)}{b_0(z_0)} \right| \le \binom{n}{m} d^{-m}$ into $|b_0(z_0)| = \sum_{k=1}^{n} |b_k(z_0)| \rho^k$ and find

$$1 = \sum_{k=1}^{n} \frac{|b_k(z_0)|}{|b_0(z_0)|} \rho^k \le \sum_{k=1}^{n} \binom{n}{k} \left(\frac{\rho}{d} \right)^k = \left(1 + \frac{\rho}{d} \right)^n - 1$$

such that $d \le \frac{\rho}{2^{1/n}-1}$. Given the solution ρ of $|b_0(z_0)| = \sum_{k=1}^{n} |b_k(z_0)| \rho^k$, the disk around z_0 with radius $\frac{\rho}{2^{1/n}-1}$ contains at least one zero of $p_n(z)$.

There exist theorems, for which we refer to Henrici (1974, pp. 457–462), that give conditions for the radius of a disk to enclose at least m zeros.

229. If $a_0 > a_1 > \cdots > a_n > 0$, then the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ does not have a zero in the unit disc $|z| \le 1$ nor on the positive real axis.

Proof: If $z = r$ is real and positive, $p_n(r) > 0$. For the other cases where $z = re^{i\theta}$ and $\theta \ne 0$, consider

$$|(1-z)p_n(z)| = \left| a_0 - \left(\sum_{k=1}^{n} (a_{k-1} - a_k) z^k + a_n z^{n+1} \right) \right|$$

$$\ge a_0 - \left| \sum_{k=1}^{n} (a_{k-1} - a_k) z^k + a_n z^{n+1} \right|$$

Further, with $r \leq 1$,

$$\left| \sum_{k=1}^{n} (a_{k-1} - a_k) z^k + a_n z^{n+1} \right| = \left| \sum_{k=1}^{n} (a_{k-1} - a_k) r^k e^{ik\theta} + a_n r^{n+1} e^{i(n+1)\theta} \right|$$

$$< \sum_{k=1}^{n} (a_{k-1} - a_k) + a_n = a_0$$

where the inequality stems from the fact that not all arguments $e^{ik\theta}$ are equal (since $\theta \neq 0$). Hence, $|(1-z)p_n(z)| > 0$ for $|z| \leq 1$. $\qquad \square$

Art. 229 also holds for a polynomial with alternating coefficients, $t_n(z) = \sum_{k=0}^{n}(-1)^k a_k z^k$, where $a_0 > a_1 > \cdots > a_n > 0$, because a zero x of $t_n(z)$ is also a zero of $p_n(-z)$ for which $|-x| > 1$. If $a_n > a_{n-1} > \cdots > a_0 > 0$, then all the zeros of the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ lie within the unit disc $|z| < 1$. This case is a consequence of **art.** 229 and **art.** 196. We refer to Milovanović *et al.* (1994) for extensions.

230. *If the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ has real, positive coefficients, then all its zeros lie in the annulus* $\min_{1 \leq k \leq n} \left(\frac{a_{k-1}}{a_k} \right) \leq |z| \leq \max_{1 \leq k \leq n} \left(\frac{a_{k-1}}{a_k} \right)$.

Proof: Consider $p_n\left(\frac{z}{x} \right) = \sum_{k=0}^{n} a_k x^{-k} z^k$ and we can always choose x such that $a_k x^{-k} < a_{k-1} x^{1-k}$ for each $1 \leq k \leq n$. Indeed, it suffices that $x^{-1} < \frac{a_{k-1}}{a_k}$ for each k or that $x^{-1} = \min_{1 \leq k \leq n} \left(\frac{a_{k-1}}{a_k} \right)$. For those x, **art.** 229 shows that $\left| p_n\left(\frac{z}{x} \right) \right| > 0$ for $|z| \leq 1$, which implies that $p_n(z)$ has no zeros within the disc with radius x^{-1}, thus $|z_k| > x^{-1}$. Applying the same method to $z^n p_n\left(\frac{y}{z} \right) = \sum_{k=0}^{n} a_{n-k} y^{n-k} z^k$ and choose y such that $a_{n-k} y^{n-k} < a_{n-k+1} y^{n-k+1}$ for each $1 \leq k \leq n$, or $y = \max_{1 \leq k \leq n} \left(\frac{a_{k-1}}{a_k} \right)$. For those y, **art.** 229 indicates that $\left| p_n\left(\frac{y}{z} \right) \right| > 0$ for $|z| \leq 1$, which implies that all zeros of $z^n p_n\left(\frac{1}{z} \right)$ lie outside the disk with radius y. In view of **art.** 196, the zeros z_k of $p_n(z)$ lie within that disc with radius y, thus $|z_k| < y$. Combining both bounds completes the proof. $\qquad \square$

231. *Weierstrass's iterative method.* Let w_j be an approximation to the zero z_j of the polynomial $p_n(z)$. The new update $\hat{w}_j = w_j + \Delta w_j$ is ideally equal to z_j, so that $p_n(\hat{w}_j) = 0$. By Taylor's Theorem, we have

$$p_n(\hat{w}_j) = p_n(w_j + \Delta w_j) = p_n(w_j) + p_n'(w_j) \Delta w_j + O\left((\Delta w_j)^2 \right)$$

Requiring that $p_n(\hat{w}_j) = 0$ and ignoring second order terms leads to the Newton Raphson rule for the increment

$$\Delta w_j = -\frac{p_n(w_j)}{p_n'(w_j)} \tag{9.35}$$

When the approximation w_j is indeed sufficiently close to z_j, subsequent iterations $w_j^{(k+1)} = w_j^{(k)} + \Delta w_j^{(k)}$ converge quadratically in k to z_j.

Weierstrass argues similarly. Ideally, all $\hat{w}_j = z_j$ for all zeros $1 \leq j \leq n$ such that the product form (9.1) of the polynomial equals

$$p_n(z) = a_n \prod_{j=1}^{n} (z - w_j + \Delta w_j)$$

Applying Taylor's Theorem to expand the n dimensional function $p_n(z; z_1, \ldots, z_n)$ in the vector $(z_1, z_2, \ldots, z_n)$ around the vector $(w_1, w_2, \ldots, w_n)$ yields

$$p_n(z) = p_n(z; w_1, \ldots, w_n) + \sum_{j=1}^{n} \left. \frac{\partial p_n(z)}{\partial z_j} \right|_{z_j = w_j} \Delta w_j + r$$

where the remainder r contains higher order terms in Δw_j such as $(\Delta w)^T H \Delta w$, where H is the Hessian. Ignoring the remainder as in Newton Raphson's rule and computing the derivative yields

$$p_n(z) \simeq a_n \prod_{j=1}^{n} (z - w_j) - a_n \sum_{j=1}^{n} \prod_{k=1; k \neq j}^{n} (z - w_k) \Delta w_j$$

All increments Δw_j for $1 \leq j \leq n$ are solved from this relation by subsequently letting $z = w_m$ for $1 \leq m \leq n$, resulting in

$$p_n(w_m) \simeq -a_n \sum_{j=1}^{n} \Delta w_j \prod_{k=1; k \neq j}^{n} (w_m - w_k) = -a_n \Delta w_m \prod_{k=1; k \neq m}^{n} (w_m - w_k)$$

from which Weierstrass' increments for $1 \leq m \leq n$ are obtained:

$$\Delta w_m = \frac{-p_n(w_m)}{a_n \prod_{k=1; k \neq m}^{n} (w_m - w_k)} \tag{9.36}$$

Iterations of $w_m^{(k+1)} = w_m^{(k)} + \Delta w_m^{(k)}$ for $1 \leq m \leq n$ in $k = 0, 1, \ldots$ converge also quadratically in k to all the $1 \leq m \leq n$ zeros z_m under much milder conditions than the Newton Raphson rule. McNamee (2007) demonstrates that Weierstrass's scheme nearly always converges, irrespective of the initial guesses $w_m^{(0)}$ for $1 \leq m \leq n$.

There is an interesting alternative derivation of the Weierstrass increments (9.36). The application of the Newton Raphson rule (9.35) to the coefficients (9.6) of Vieta's formula expressed in terms of the zeros yields a set of linear equations in Δw_m that leads to (9.36). The simplest linear equation, $\frac{a_{n-1}}{a_n} = -\sum_{k=1}^{n} z_k$ for $k = n - 1$ in (9.6), is already linear in $z_k = \hat{w}_k = w_k + \Delta w_k$ and shows that, at each iteration $\sum_{m=1}^{n} w_m^{(k+1)} = -\frac{a_{n-1}}{a_n}$, meaning that the sum of approximations equals the exact sum.

Just as there are many improvements of the Newton Raphson rule to enhance the convergence towards the root, so are there many variants that improve Weierstrass's rule. Moreover, there are conditions for the initial values $w_m^{(0)}$ to guarantee convergence, which are discussed in McNamee (2007).

9.8 Zeros of complex functions

232. *The argument principle.*

Theorem 58 *If $f(z)$ is analytic on and inside the contour C, then the number of zeros of $f(z)$ inside C is*

$$N = \frac{1}{2\pi i} \int_C \frac{f'(z)}{f(z)} dz = \frac{1}{2\pi} \Delta_C \arg f(z)$$

where Δ_C denotes the variation of the argument of f round the contour C.

Proof: See Titchmarsh (1964, p. 116). □

Since polynomials are analytic in the entire complex plane, Theorem 58 is valid for any contour C and can be used to compute the number of zeros inside a certain contour as shown in Section 9.6.

233. The famous and simple theorems of Rouché and of Jensen are very powerful tools in complex analysis.

Theorem 59 (Rouché) *If $f(z)$ and $g(z)$ are analytic inside and on a closed contour C, and $|g(z)| < |f(z)|$ on C, then $f(z)$ and $f(z) + g(z)$ have the same number of zeros inside C.*

Proof: See Titchmarsh (1964, p. 116). □

If at all points of a contour C around the origin holds that

$$|a_k z^k| > \left| \sum_{j=0; j \neq k}^{n} a_j z^j \right|$$

then the contour C encloses k zeros of $p_n(z) = \sum_{k=0}^{n} a_k z^k$.

Proof: A proof not directly based on Rouché's Theorem is given in Whittaker and Watson (1996, p. 120). The result directly follows from Rouché's Theorem 59 with $f(z) = a_k z^k$, which has a k multiple zero at the origin and $g(z) = \sum_{j=0; j \neq k}^{n} a_j z^j$. □

We give another application of Rouché's Theorem to a polynomial $p_n(z)$ with real coefficients $a_0 > a_1 > \cdots > a_n > 0$. If R is such that $a_0 > \sum_{k=1}^{n} a_k R^k$, then $p_n(z)$ has no zeros in the disk around the origin with radius R. If $R > 1$, an improvement of **art.** 229 is obtained.

Theorem 60 (Jensen) *Let $f(z)$ be analytic for $|z| < R$. Suppose that $f(0) \neq 0$, and let $r_1 \leq r_2 \leq \ldots \leq r_n \leq \ldots$ be the moduli of the zeros of $f(z)$ in the circle $|z| < R$. Then, if $r_n \leq r \leq r_{n+1}$,*

$$n \log r + \log |f(0)| - \sum_{j=1}^{n} \log r_j = \frac{1}{2\pi} \int_0^{2\pi} \log \left| f\left(re^{i\theta}\right) \right| d\theta$$

Proof: See Titchmarsh (1964, p. 125).   □

Consider the polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ with zeros, ordered as $|z_1| > |z_2| > \ldots > |z_m| > 1 \geq |z_{m+1}| > \ldots > |z_n|$. Assuming that $a_0 \neq 0$, then Jensen's Theorem 60 states for $r = 1$ that

$$\log \frac{|a_0|}{\prod_{j=m+1}^{n} |z_j|} = \frac{1}{2\pi} \int_0^{2\pi} \log \left| p_n \left(e^{i\theta} \right) \right| d\theta$$

Using $a_0 = (-1)^n a_n \prod_{k=1}^{n} z_k$ in **art.** 196 yields

$$\frac{1}{2\pi} \int_0^{2\pi} \log \left| p_n \left(e^{i\theta} \right) \right| d\theta = \log |a_n| \prod_{k=1}^{m} |z_k| \tag{9.37}$$

With

$$\left| p_n \left(e^{i\theta} \right) \right| = \left| \sum_{k=0}^{n} a_k e^{ik\theta} \right| \leq \sum_{k=0}^{n} |a_k|$$

we obtain the inequality of Mahler (1960),

$$|a_n| \prod_{k=1}^{m} |z_k| \leq \sum_{k=0}^{n} |a_k| \tag{9.38}$$

Recall that, if all coefficients $\{a_k\}_{0 \leq k \leq n}$ of the polynomial $p_n(z)$ are real, then $\prod_{k=1}^{m} |z_k| = (-1)^l \prod_{k=1}^{m} z_k$, where l is the number of real negative zeros. Mahler (1960) also derives a lower bound for $|a_n| \prod_{k=1}^{m} |z_k|$. Let $1 \leq j_k \leq n$, then, for any $0 \leq k \leq n$,

$$\prod_{i=1}^{k} |z_{j_i}| \leq \prod_{l=1}^{m} |z_l|$$

Vieta's formula (9.6) shows that, for each $0 \leq k \leq n$,

$$\left| \frac{a_{n\ k}}{a_n} \right| = \left| \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_k=j_{k\ 1}+1}^{n} \prod_{i=1}^{k} z_{j_i} \right| \leq \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_k=j_{k\ 1}+1}^{n} \left| \prod_{i=1}^{k} z_{j_i} \right|$$

$$\leq \prod_{l=1}^{m} |z_l| \sum_{j_1=1}^{n} \sum_{j_2=j_1+1}^{n} \cdots \sum_{j_k=j_{k\ 1}+1}^{n} 1 = \binom{n}{k} \prod_{l=1}^{m} |z_l|$$

Multiplying by $\rho^{n\ k}$ and summing over all k results in

$$\sum_{k=0}^{n} |a_{n\ k}| \rho^{n\ k} = \sum_{k=0}^{n} |a_k| \rho^k \leq |a_n| \prod_{l=1}^{m} |z_l| \sum_{k=0}^{n} \binom{n}{k} \rho^{n\ k} = (1+\rho)^n |a_n| \prod_{l=1}^{m} |z_l|$$

which gives Mahler's lower bound when $\rho = 1$,

$$(1+\rho)^{\ n} \sum_{k=0}^{n} |a_k| \rho^k \leq |a_n| \prod_{l=1}^{m} |z_l| \tag{9.39}$$

234. *Lagrange's series for the inverse of a function.* Let the function $w = f(z)$ be analytic around the point z_0 and $f'(z_0) \neq 0$. Then, there exists a region around $w_0 = f(z_0)$, in which each point has a unique inverse $z = f^{-1}(w)$ belonging to the analytic region around z_0. The Lagrange series for the inverse of a function (Markushevich, 1985, II, pp. 88),

$$f^{-1}(w) = z_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\frac{d^{n-1}}{dz^{n-1}} \left(\frac{z - z_0}{f(z) - f(z_0)} \right)^n \right] \Bigg|_{z=z_0} (w - f(z_0))^n \qquad (9.40)$$

is a special case (for $G(z) = z$) of the more general result

$$G(f^{-1}(w)) = G(z_0) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\frac{d^{n-1}}{dz^{n-1}} G'(z) \left(\frac{z - z_0}{f(z) - f(z_0)} \right)^n \right] \Bigg|_{z=z_0} (w - f(z_0))^n \qquad (9.41)$$

Provided that $G(z)$ is analytic inside the contour C around z_0, that encloses a region where $f(z) - w_0$ has only a single zero, then the last series (9.41) follows from expanding the integral

$$G(f^{-1}(w)) = \frac{1}{2\pi i} \int_C G(z) \frac{f'(z)}{f(z) - w} \, dz$$

in a Taylor series around $w_0 = f(z_0)$,

$$G(f^{-1}(w)) = \sum_{n=0}^{\infty} \left[\frac{1}{2\pi i} \int_C G(z) \frac{f'(z)}{(f(z) - f(z_0))^{n+1}} \, dz \right] (w - f(z_0))^n$$

Applying integration by parts for $n > 0$ gives

$$\frac{1}{2\pi i} \int_C G(z) \frac{f'(z)}{(f(z) - f(z_0))^{n+1}} \, dz = -\frac{1}{2\pi i n} \int_C G(z) d \left(\frac{1}{(f(z) - f(z_0))^n} \right) dz$$
$$= \frac{1}{2\pi i n} \int_C \frac{G'(z)}{(f(z) - f(z_0))^n} \, dz$$

After rewriting,

$$\frac{1}{2\pi i} \int_C \frac{G'(z)}{(f(z) - f(z_0))^n} \, dz = \frac{1}{2\pi i} \int_C \left(\frac{(z - z_0)}{(f(z) - f(z_0))} \right)^n \frac{G'(z)}{(z - z_0)^n} \, dz$$

and invoking Cauchy's integral formula (9.23) for the k th derivative, we obtain (9.41).

A zero ζ of a function $w = f(z)$, whose inverse is $z = f^{-1}(w)$, satisfies $\zeta = f^{-1}(0)$. If the Taylor series $f(z) = \sum_{k=0}^{\infty} f_k(z_0)(z - z_0)^k$ is known, the Lagrange series (9.40) can be computed formally using characteristic coefficients (Van Mieghem, 2007) to any desired order. Explicitly, up to order five in $\frac{f_0(z_0)}{f_1(z_0)}$, we

have

$$\zeta(z_0) \approx z_0 - \frac{f_0(z_0)}{f_1(z_0)} - \frac{f_2(z_0)}{f_1(z_0)} \left(\frac{f_0(z_0)}{f_1(z_0)}\right)^2 + \left[-2\left(\frac{f_2(z_0)}{f_1(z_0)}\right)^2 + \frac{f_3(z_0)}{f_1(z_0)}\right]\left(\frac{f_0(z_0)}{f_1(z_0)}\right)^3$$

$$+ \left[-5\left(\frac{f_2(z_0)}{f_1(z_0)}\right)^3 + 5\frac{f_3(z_0)}{f_1(z_0)}\frac{f_2(z_0)}{f_1(z_0)} - \frac{f_4(z_0)}{f_1(z_0)}\right]\left(\frac{f_0(z_0)}{f_1(z_0)}\right)^4$$

$$+ \left[-14\left(\frac{f_2(z_0)}{f_1(z_0)}\right)^4 + 21\frac{f_3(z_0)}{f_1(z_0)}\left(\frac{f_2(z_0)}{f_1(z_0)}\right)^2 - 3\left(\frac{f_3(z_0)}{f_1(z_0)}\right)^2\right.$$

$$\left. -6\frac{f_4(z_0)}{f_1(z_0)}\frac{f_2(z_0)}{f_1(z_0)} + \frac{f_5(z_0)}{f_1(z_0)}\right]\left(\frac{f_0(z_0)}{f_1(z_0)}\right)^5 \tag{9.42}$$

from which we observe that the two first terms are Newton Raphson's correction (9.35) in **art.** 231. The formal Lagrange expansion, where only a few terms in (9.42) are presented, only converges provided z_0 is chosen sufficiently close to the zero $\zeta(z_0)$, which underlines the importance of the choice for z_0. Another observation is that, if all Taylor coefficients $f_k(z_0)$ are real as well as z_0, the Lagrange series only possesses real terms such that the zero $\zeta(z_0)$ is real. Thus, for any polynomial $f(z) = p_n(z)$ with given real coefficients, a converging Lagrange series for some real z_0 identifies a real zero $\zeta(z_0)$.

9.9 Bounds on values of a polynomial

Milovanović *et al.* (1994) have collected a large amount of bounds on values of a polynomial of several types. Here, we only mention the first contributions to field by Pavnuty Chebyshev.

235. Chebyshev proved the following theorem:

Theorem 61 (Chebyshev) *Let $p_n(x) = \sum_{k=0}^{n} a_k x^k$ be a polynomial with real coefficients and $a_n = 1$, then, for $n \geq 1$,*

$$\max_{1 \leq x \leq 1} |p_n(x)| \geq \frac{1}{2^{n-1}}$$

The equality sign is obtained for $p_n(z) = \frac{T_n(z)}{2^{n-1}}$, where $T_n(z) = \cos(n \arccos z)$ are the Chebyshev polynomials of the first kind.

Proof: See, e.g., Aigner and Ziegler (2003, Chapter 18). □

An immediate consequence is:

Corollary 2 *For a real and monic polynomial $p_n(z)$, suppose that $|p_n(x)| \leq c$ for all $x \in [a, b]$. Then, $b - a \leq 4\left(\frac{c}{2}\right)^{1/n}$.*

Proof: We map the x interval $[a, b]$ onto the y interval $[-1, 1]$ by the linear transform $y = \frac{2}{b-a}(x-a) - 1$. The corresponding polynomial

$$q_n(y) = p_n\left(\frac{b-a}{2}(y+1) + a\right)$$

has leading coefficient $\left(\frac{b-a}{2}\right)^n$ and satisfies

$$\max_{1 \leq y \leq 1} |q_n(y)| = \max_{a \leq x \leq b} |p_n(x)|$$

By Chebyshev's Theorem 61 we deduce that $\max_{1 \leq y \leq 1} |q_n(y)| \geq \left(\frac{b-a}{2}\right)^n \frac{1}{2^{n-1}} = 2\left(\frac{b-a}{4}\right)^n$. Hence,

$$2\left(\frac{b-a}{4}\right)^n \leq \max_{a \leq x \leq b} |p_n(x)| \leq c$$

such that $b - a \leq 4\left(\frac{c}{2}\right)^{1/n}$. $\square$

9.10 Bounds for the spacing between zeros

236. *Minimum distance between zeros.* Mahler (1964) proved a beautiful theorem that bounds the minimum spacing or distance between any pair of simple zeros of a polynomial. Only if all zeros are simple or distinct, the discriminant $\Delta(p_n)$ is non zero as shown in **art.** 201. Moreover, Mahler's lower bound (9.43) is the best possible.

Theorem 62 (Mahler) *For any polynomial $p_n(x)$ with degree $n \geq 2$ and distinct zeros, ordered as $|z_1| > |z_2| > \ldots > |z_m| > 1 \geq |z_{m+1}| > \ldots > |z_n|$, the minimum distance between any pair of zeros is bounded from below by*

$$\min_{1 \leq k < j \leq n} |z_k - z_j| > \frac{\sqrt{3|\Delta(p_n)|}}{n^{\frac{n}{2}+1}\left(|a_n|\prod_{j=1}^{m}|z_j|\right)^{n-1}} \geq \frac{\sqrt{3|\Delta(p_n)|}}{n^{\frac{n}{2}+1}\left(\sum_{k=0}^{n}|a_k|\right)^{n-1}} \qquad (9.43)$$

*where $\Delta(p_n)$ is the discriminant, defined in **art.** 201.*

Proof: The relation (9.11) between the discriminant and the Vandermonde determinant suggests us to start considering the Vandermonde matrix $V_n(z)$ in (8.90) of the zeros, ordered as in Theorem 62. Subtract row s from row r and use the algebraic formula $x^k - y^k = (x-y)\sum_{j=0}^{k-1} x^{k-1-j}y^j$ such that

$$\det V_n\left(z\right) = \left(z_r - z_s\right)\begin{bmatrix} 1 & z_1 & z_1^2 & z_1^3 & \cdots & z_1^{n-1} \\ 1 & z_2 & z_2^2 & z_2^3 & \cdots & z_2^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & z_r + z_s & z_r^2 + z_r z_s + z_s^2 & \cdots & \sum_{j=0}^{n-2} z_r^{n-2-j} z_s^j \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & z_n & z_n^2 & z_n^3 & \cdots & z_n^{n-1} \end{bmatrix}$$

We now proceed similarly as in **art. 195** by dividing the first m rows, corresponding to the components with absolute value larger than 1, by z_j^{n-1} for $1 \le j \le m$. The only difference lies in row r, that consists of the elements

$$\begin{array}{cccccc} 0 & 1 & z_r + z_s & z_r^2 + z_r z_s + z_s^2 & \cdots & \sum_{j=0}^{n-2} z_r^{n-2-j} z_s^j & \text{if } r > m \\ 0 & z_r^{-(n-2)} & \frac{z_r + z_s}{z_r^{n-1}} & \frac{z_r^2 + z_r z_s + z_s^2}{z_r^{n-1}} & \cdots & \frac{\sum_{j=0}^{n-2} z_r^{n-2-j} z_s^j}{z_r^{n-1}} & \text{if } r \le m \end{array}$$

Since $r < s$, the ordering tells us that $|z_r| > |z_s|$. If $r > m$, then $1 \ge |z_r| > |z_s|$, and the k-th element in row r is bounded by $\left|\sum_{j=0}^{k-2} z_r^{k-2-j} z_s^j\right| \le k - 1$, while if $r \le m$, then $|z_r| > 1$ such that k-th element in row r is bounded by $\left|\sum_{j=0}^{k-2} \frac{z_r^{k-2-j} z_s^j}{z_r^{n-1}}\right| \le k-1$. Hadamard's inequality (8.93) shows that

$$\left|\det V_n\left(z\right)\right| \le \left|z_r - z_s\right| n^{\frac{n-1}{2}} \prod_{j=1}^{m} |z_j|^{n-1} \sqrt{\sum_{k=1}^{n} (k-1)^2}$$

Using $\sum_{k=1}^{n-1} k^2 = \frac{n(n-1)(2n-1)}{6} < \frac{n^3}{3}$ (Abramowitz and Stegun, 1968, Section 23.1.4), we have

$$\left|\det V_n\left(z\right)\right| \le \frac{\left|z_r - z_s\right|}{\sqrt{3}} n^{\frac{n+2}{2}} \prod_{j=1}^{m} |z_j|^{n-1} \tag{9.44}$$

This inequality (9.44) is nearly the best possible, because equality is attained if $z_j = e^{2\pi i \frac{j}{n}}$ as shown in **art. 195** and **art. 143**. Choosing $z_r = 1$ and $z_s = e^{\frac{2\pi i}{n}}$, $|z_r - z_s| = 2 \sin\frac{\pi}{n}$, while we know from (8.94) that $|\det V_n\left(z\right)| = n^{n/2}$ such that $\frac{|\det V_n(z)|}{|z_r - z_s|} = \frac{n^{n/2}}{2\sin\frac{\pi}{n}} = \frac{\frac{\pi}{n}}{\sin\frac{\pi}{n}}\left(\frac{n^{\frac{n+2}{2}}}{2\pi}\right)$, which tends to $\frac{|\det V_n(z)|}{|z_r - z_s|} \to \frac{n^{\frac{n+2}{2}}}{2\pi}$ for large n. This illustrates that (9.44) cannot be improved, except perhaps for a slightly smaller prefactor than $\frac{1}{\sqrt{3}}$. Since the inequality (9.44) holds for any r and s, Theorem 62 now follows from the definition of the discriminant (9.11). The last inequality in (9.43) follows from (9.38). $\qquad\square$

Usually, the discriminant $\Delta\left(p_n\right)$ is not easy to determine. However, for a poly nomial with integer coefficients (and thus also rational coefficients because $\frac{p_n(z)}{\alpha}$ and $p_n\left(z\right)$ have the same zeros for any complex number $\alpha \ne 0$), **art. 201** shows that $\Delta\left(p_n\right)$ is a function of the coefficients a_k and, hence, an integer. In addition

$\Delta(p_n) \neq 0$, such that $|\Delta(p_n)| \geq 1$. Thus, the minimum spacing between the simple zeros of a polynomial with rational coefficients $a_k \in \mathbb{Q}$ is lower bounded by

$$\min_{1 \leq k < j \leq n} |z_k - z_j| > \frac{\sqrt{3}}{n^{\frac{n}{2}+1} \left(\sum_{k=0}^{n} |a_k|\right)^{n-1}} \tag{9.45}$$

237. An upper bound for the spacing (Milovanović *et al.*, 1994, p. 106) due to Lupas is

$$\min_{1 \leq k < j \leq n} |z_k - z_j| \leq 2\sqrt{\frac{3 \operatorname{Var}[z]}{n^2 - 1}}$$

where the variance of the zeros of a real polynomial is defined as

$$\operatorname{Var}[z] = \frac{1}{n} \sum_{k=1}^{n} z_k^2 - \left(\frac{1}{n} \sum_{k=1}^{n} z_k\right)^2$$

Using the Newton identities in **art.** 198 yields

$$\operatorname{Var}[z] = \frac{1}{n^2} \left\{ (n-1) \frac{a_{n-1}^2}{a_n^2} - \frac{2n a_{n-2}}{a_n} \right\}$$

Equality in the upper bound is attained for the polynomial

$$p_n(z) = \prod_{k=1}^{n} \left(z - E[z] - (n - 2k + 1) \sqrt{\frac{3 \operatorname{Var}[z]}{n^2 - 1}} \right)$$

where the mean of the zeros $E[z] = \frac{1}{n} \sum_{k=1}^{n} z_k = -\frac{a_{n-1}}{n a_n}$.

9.11 Bounds on the zeros of a polynomial

McNamee (2007) provides a long list of bounds on the modulus of the largest zero $\zeta = \max_{1 \leq k \leq n} |z_k|$ of $p_n(z)$, where the coefficients $a_k \in \mathbb{C}$ and $a_n = 1$. By testing over a large number of polynomials, he mentions that the relatively simple formula, due to Deutsch (1970),

$$\zeta \leq |a_{n-1}| + \max_{1 \leq k \leq n-1 \text{ and } a_k \neq 0} \left| \frac{a_{k-1}}{a_k} \right|$$

which is an extension of **art.** 196 to complex coefficients a_k derived from the companion matrix (**art.** 143) using matrix norms, ended up as second best. The best one, due to Kalantari,

$$\zeta \leq \max_{4 \leq k \leq n+3} \left| a_{n-1}^2 a_{n-k+3} - a_{n-1} a_{n-k+2} - a_{n-2} a_{n-k+3} + a_{n-k+1} \right|^{\frac{1}{k-1}}$$

is clearly more complicated.

238. Let z_1 denote the zero with largest modulus and define $\sigma_j = \sum_{k=1}^{n} |z_k|^j \geq |Z_j|$. Evidently, $|z_1|^j \leq \sigma_j$. On the other hand, since $|z_1| \geq |z_k|$ for any $1 \leq k \leq n$,

$$\sigma_{j+1} = \sum_{k=1}^{n} |z_k|^j |z_k| \leq |z_1| \sum_{k=1}^{n} |z_k|^j = |z_1| \sigma_j$$

Combining both inequalities yields the bounds, for any $j > 0$,

$$\frac{\sigma_{j+1}}{\sigma_j} \leq |z_1| \leq \sigma_j^{\frac{1}{j}}$$

239. The Hölder inequality, presented in **art.** 8.40 in vector form is, with $p > 1$ and $\frac{1}{p} + \frac{1}{q} = 1$,

$$\sum_{j=1}^{n} |x_j y_j| \leq \left(\sum_{j=1}^{n} |x_j|^p \right)^{\frac{1}{p}} \left(\sum_{j=1}^{n} |y_j|^q \right)^{\frac{1}{q}} \tag{9.46}$$

Quite likely, there exists a value of $p > 1$ that results in the lowest upper bound, but that value of p will dependent on the values of x_j and y_j. For any integer m and j, we may write

$$\sigma_j = \sum_{k=1}^{n} \left| z_k^{j-m} \right| |z_k^m|$$

Applying (9.46) gives

$$\sigma_j \leq \left(\sum_{k=1}^{n} |z_k|^{p(j-m)} \right)^{\frac{1}{p}} \left(\sum_{k=1}^{n} |z_k|^{\frac{pm}{p-1}} \right)^{1-\frac{1}{p}}$$

where we require that $p(j - m) = l$ and $\frac{pm}{p-1} = h$ and both l and m are integers. All solutions satisfy $m(l - h) = (l - j)h$ with $l > 0$ and $p = \frac{l}{j-m}$. For example, the solution $h = l = j$ and $p = \frac{j}{j-m}$ returns, for any m and j, an equality, namely the definition of σ_j. The case $p = 2$ is

$$\sigma_j^2 \leq \left(\sum_{k=1}^{n} |z_k|^{2(j-m)} \right) \left(\sum_{k=1}^{n} |z_k|^{2m} \right) = \sigma_{2(j-m)} \sigma_{2m} \tag{9.47}$$

which is particularly useful in the case where j is even and all zeros are real.

240. The next theorem sharpens the bounds in **art.** 238:

Theorem 63 *If $z_1, \ldots, z_n$ are the real zeros of a polynomial $p_n(z) = \sum_{k=0}^{n} a_k z^k$ for which $Z_1 = \sum_{k=1}^{n} z_k = 0$, then any zero $\zeta \in \{z_1, \ldots, z_n\}$ is bounded, for positive integers $1 \leq m \leq \left[\frac{n}{2} \right]$ by*

$$- \left(\frac{Z_{2m}}{1 + \frac{1}{(N-1)^{2m-1}}} \right)^{\frac{1}{2m}} \leq \zeta \leq \left(\frac{Z_{2m}}{1 + \frac{1}{(N-1)^{2m-1}}} \right)^{\frac{1}{2m}} \tag{9.48}$$

where $Z_j = \sum_{k=1}^N z_k^j$ is uniquely expressed via the recursion (9.4) in terms of the coefficients a_k.

Before proving Theorem 63, we note that, as shown in **art. 203**, the condition $Z_1 = 0$, which is equivalent to the requirement that $a_{n-1} = 0$ by (9.5), is not confining.

Proof: Let z_1 denote an arbitrary zero of $p_n(z)$ (because we can always relabel the zeros), then

$$Z_j = z_1^j + \sum_{k=2}^n z_k^j$$

Applying the Hölder inequality (9.46) to $x_j = 1$ and $y_j = z_j \in \mathbb{R}$ for $2 \leq j \leq n$, yields for even $q = 2m$,

$$\frac{1}{(n-1)^{2m-1}} \left(\sum_{j=2}^n |z_j| \right)^{2m} \leq \sum_{k=2}^n z_k^{2m} \tag{9.49}$$

Since $\sum_{j=2}^n z_j \leq \sum_{j=2}^n |z_j|$ and $\sum_{j=2}^n z_j = -\frac{a_{n-1}}{a_n} - z_1$, the inequality (9.49) becomes

$$\frac{1}{(n-1)^{2m-1}} \left(\frac{a_{n-1}}{a_n} + z_1 \right)^{2m} \leq Z_{2m} - z_1^{2m} \tag{9.50}$$

Using the assumption that $a_{n-1} = 0$, we finally arrive, for all $1 \leq m \leq \left[\frac{n}{2}\right]$, at our bounds (9.48) for any zero of $p_n(z)$, and thus also for the largest zero. $\qquad\square$

Theorem 63 actually generalizes a famous theorem due to Laguerre in which $m = 1$ and where the condition that $Z_1 = 0$ was not needed.

Theorem 64 (Laguerre) *If all the zeros $z_1, \ldots, z_n$ of a polynomial $p_n(x) = \sum_{k=0}^n a_k x^k$ with $a_n = 1$ are real, then they all lie in the interval $[y_-, y_+]$ where*

$$y_\pm = -\frac{a_{n-1}}{n} \pm \frac{n-1}{n} \sqrt{a_{n-1}^2 - \frac{2n}{n-1} a_{n-2}}$$

Proof: Laguerre's theorem follows immediately from (9.50) and the Newton identities in **art. 198** for $m = 1$. See also Aigner and Ziegler (2003, p. 101). $\qquad\square$

Since the quartic equation ($m = 2$ in (9.50)) is still solvable exactly, that case can be expressed in closed form without using the condition $Z_1 = 0$, as in the proof of Laguerre's Theorem 64. However, all other $m \geq 2$ cases are greatly simplified by the condition $Z_1 = 0$, that relieves us from solving a polynomial equation of order $2m$.

Theorem 65 *If $z_1, \ldots, z_n$ are the real zeros of a polynomial $p_n(z) = \sum_{k=0}^n a_k z^k$,*

then any zero $\zeta \in \{z_1, \ldots, z_n\}$ is upper bounded, for positive integers m, by

$$z_1 \leq \left(\frac{Z_{2m}}{n} + \sqrt{(n-1)} \sqrt{\frac{Z_{4m}}{n} - \left(\frac{Z_{2m}}{n} \right)^2} \right)^{\frac{1}{m}} \tag{9.51}$$

and lower bounded for odd integer values of m, by

$$z_1 \geq \left(\frac{Z_{2m}}{n} - \sqrt{(n-1)} \sqrt{\frac{Z_{4m}}{n} - \left(\frac{Z_{2m}}{n} \right)^2} \right)^{\frac{1}{m}} \tag{9.52}$$

Proof: In a similar vein, application of (9.47) for $j = 2m$ and $m = l$, gives

$$\left(Z_{2m} - z_1^{2m} \right)^2 \leq \left(Z_{2(2m-l)} - z_1^{2(2m-l)} \right) \left(Z_{2l} - z_1^{2l} \right)$$

or

$$Z_{2m}^2 - 2z_1^{2m} Z_{2m} \leq Z_{4m-2l} Z_{2l} - z_1^{2l} Z_{4m-2l} - z_1^{4m-2l} Z_{2l}$$

If $l = m$, then the dependence on z_1 disappears. If $l = \frac{m}{2}$ or $l = \frac{3m}{2}$, then

$$z_1^{3m} Z_m - 2z_1^{2m} Z_{2m} + z_1^m Z_{3m} + Z_{2m}^2 - Z_{3m} Z_m \leq 0$$

whose exact solution (via Cardano's formula) is less attractive. For $l = 0$, the quadratic inequality in z_1^m

$$z_1^{4m} - \frac{2Z_{2m}}{n} z_1^{2m} + \frac{Z_{2m}^2 - (n-1) Z_{4m}}{n} \leq 0$$

is obeyed for any z_1^m lying in between

$$z_{\pm} = \frac{Z_{2m}}{n} \pm \sqrt{(n-1)} \sqrt{\frac{Z_{4m}}{n} - \left(\frac{Z_{2m}}{n} \right)^2}$$

The Cauchy Schwarz inequality (8.41) shows that $\frac{Z_{4m}}{n} - \left(\frac{Z_{2m}}{n} \right)^2 \geq 0$, implying that the roots are real. Thus, we find the upper bound (9.51) and the lower bound (9.52), that always exists for odd m. $\qquad\square$

10

Orthogonal polynomials

The classical theory of orthogonal polynomials is reviewed from an algebraic point of view. The book by Szegő (1978) is still regarded as the standard text, although it approaches the theory of orthogonal polynomials via complex function theory and differential equations. The classical theory of orthogonal polynomials is remarkably beautiful, and powerful at the same time. Moreover, as shown in Section 5.11, we found interesting relations with graph theory.

An overview and properties of the classical orthogonal polynomials such as Legendre, Chebyshev, Jacobi, Laguerre and Hermite polynomials is found in Abramowitz and Stegun (1968, Chapter 22). A general classification scheme of orthogonal polynomials is presented by Koekoek *et al.* (2010). The theory of expanding an arbitrary function in terms of solutions of a second order differential equation, initiated by Sturm and Liouville, and treated by Titchmarsh (1962) and by Titchmarsh (1958) for partial differential equations, can be regarded as the generalization of orthogonal polynomial expansions.

10.1 Definitions

241. The usual scalar or inner product between two vectors x and y, that is denoted as $x^T y$, is generalized to real functions f and g as the Stieltjes Lebesgue integral[1] over the interval $[a, b]$

$$(f, g) = \int_a^b f(u) g(u) \, dW(u) \tag{10.1}$$

where the distribution function W is a non decreasing, non constant function in

---

[1] As mentioned in the introduction of Van Mieghem (2006b, Chapter 2), the Stieltjes integral unifies both continuous and differentiable distribution functions as well as discrete ones, in which case, the integral reduces to a sum. If W is differentiable, then

$$(f, g) \quad \int_a^b f(u) g(u) w(u) \, du$$

and the non-negative function $w(u) \quad W'(u)$ is often called a weight function. A broader discussion is given by Szegő (1978, Section 1.4).

$[a, b]$. As in linear algebra, the function f and g are called orthogonal if $(f, g) = 0$ and, likewise, the norm of f is $\|f\| = \sqrt{(f, f)}$. Moreover, the generalization (10.1) is obviously linear, $(\alpha f + \beta h, g) = \alpha (f, g) + \beta (h, g)$ and commutative $(f, g) = (g, f)$. The definition thus assumes the knowledge of both the interval $[a, b]$ as well as the distribution function W. All functions f, for which the integral $\int_a^b |f(u)|^2 \, dW(u)$ in (10.1) exists, constitute the space $L^2_{[a,b]}$.

242. An orthogonal set of real functions $f_0(x), f_1(x), \ldots, f_m(x)$ is defined, for any $k \neq l \in \{0, 1, \ldots, m\}$, by

$$(f_k, f_l) = \int_a^b f_k(u) f_l(u) \, dW(u) = 0 \tag{10.2}$$

When $(f_k, f_k) = 1$ for all $k \in \{0, 1, \ldots, m\}$, the set is normalized and called an orthonormal set of functions. Just as in linear algebra, these functions $\{f_k\}_{0 \leq k \leq m}$ are linearly independent. Since polynomials are special types of functions, an orthogonal set of polynomials $\{\pi_k\}_{0 \leq k \leq m}$ is also defined by (10.2), and we denote, an orthogonal polynomial of degree n, by π_n or $\pi_n(x)$. In addition, the general polynomial expression (9.1) is

$$\pi_n(x) = \sum_{k=0}^{n} c_{k;n} x^k \tag{10.3}$$

The special scalar product $m_k = (x^k, 1)$, or in integral form

$$m_k = \int_a^b u^k \, dW(u) \tag{10.4}$$

is called the moment of order k, and is further studied in **art.** 246.

If $\pi_n(x)$ is an orthogonal polynomial, then $\widetilde{\pi}_n(x) = \frac{\pi_n(x)}{\sqrt{(\pi_n, \pi_n)}}$ is an orthonormal polynomial. Although the highest coefficients $c_{n;n}$ can be any real number, we may always choose $c_{n;n} > 0$ since any polynomial can be multiplied by a number without affecting the zeros. The fact that $c_{n;n} > 0$ is sometimes implicitly assumed.

243. *The Gram Schmidt orthogonalization process.* Analogous to linear algebra, where a set of n linearly independent vectors that span the n dimensional space are transformed into an orthonormal set of vectors, the Gram Schmidt orthogonalization process can also be used to construct a set of orthonormal polynomials, defined by the scalar product (10.1). First, the constant polynomial of degree zero $\pi_0(x) = \pi_0$ is chosen to obey

$$1 = (\pi_0, \pi_0) = \pi_0^2 \int_a^b dW(u) = \pi_0^2 m_0$$

where the moment of order zero in (10.4) equals

$$m_0 = W(b) - W(a) > 0$$

because the distribution function $W(x)$ is non decreasing in x. Thus, $\widetilde{\pi}_0(x) = \frac{1}{\sqrt{m_0}}$.

The degree one polynomial, $\pi_1(x) = c_{1;1}x + c_{0;1}$ must be orthogonal to $\pi_0(x)$ and orthonormal, $(\pi_1, \pi_1) = 1$. These two requirements result in

$$(\pi_1, \pi_0) = c_{1;1}(x, \pi_0) + c_{0;1}(1, \pi_0) = 0$$

such that $c_{0;1} = -\frac{c_{1;1}(x,\pi_0)}{(1,\pi_0)}$, while normalization requires that $\widetilde{\pi}_1(x) = \frac{c_{1;1}x + c_{0;1}}{\sqrt{(\pi_1,\pi_1)}}$. Combined, leads to

$$\widetilde{\pi}_1(x) = \frac{c_{1;1}}{\sqrt{(\pi_1, \pi_1)}}\left(x - \frac{(x, \pi_0)}{(1, \pi_0)}\right)$$

Both π_1 and π_0 are real polynomials.

We can continue the process and compute the degree two polynomial that is orthogonal to both π_1 and π_0, and that is also orthonormal. Suppose now that we have constructed a sequence of orthonormal polynomials $\pi_0, \pi_1, \ldots, \pi_{n-1}$, which are all real, obey the orthogonality condition (10.2) and are normalized, $(\pi_k, \pi_k) = 1$. Next, we construct the polynomial $\pi_n(x)$ that is orthogonal to all lower degree orthonormal polynomials by considering

$$\pi_n(x) = c_{n;n}x^n - \sum_{k=0}^{n-1} a_k \pi_k(x)$$

Orthogonality requires for $j < n$ that

$$0 = (\pi_n, \pi_j) = c_{n;n}(x^n, \pi_j) - \sum_{k=0}^{n-1} a_k(\pi_k, \pi_j)$$

$$= c_{n;n}(x^n, \pi_j) - a_j(\pi_j, \pi_j)$$

such that

$$a_j = c_{n;n}\frac{(x^n, \pi_j)}{(\pi_j, \pi_j)}$$

After normalization $(\pi_n, \pi_n) = 1$, we obtain the real orthonormal polynomial of degree n:

$$\widetilde{\pi}_n(x) = \frac{c_{n;n}}{\sqrt{(\pi_n, \pi_n)}}\left(x^n - \sum_{k=0}^{n-1}\frac{(x^n, \pi_k)}{(\pi_k, \pi_k)}\pi_k(x)\right)$$

By induction on n, it follows that there exists an orthonormal set of polynomials belonging to the scalar product (10.1).

10.2 Properties

244. *Key orthogonality property.* Let $p_n(x)$ be an arbitrary polynomial of degree

n, then it can be written as a linear combination of the (linearly independent) orthogonal polynomials $\{\pi_k\}_{0 \le k \le m}$, provided $m \ge n$. Hence,

$$p_n(x) = \sum_{k=0}^{n} b_{k;n} \pi_k(x)$$

After multiplying both sides by $\pi_l(x)$, taking the scalar product, and using the orthogonality in (10.2), we find that, for all $0 \le l \le n$,

$$b_{l;n} = \frac{(p_n, \pi_l)}{(\pi_l, \pi_l)}$$

Hence, any polynomial of degree $n \le m$ can be expressed in a unique way as a linear combination of the set of orthogonal polynomials $\{\pi_k\}_{0 \le k \le m}$. Because $p_n(x)$ is of degree n, we notice that the coefficients $b_{l;n} = 0$ when $l > n$. In summary, a key property of orthogonality is

$$(p_n, \pi_l) = \begin{cases} b_{l;n} \|\pi_l\|^2 & \text{if } 0 \le l \le n \\ 0 & \text{if } l > n \end{cases}$$

245. *Example of* **art.** *244.* If $p_n(x) = \pi_n(x) = \sum_{k=0}^{n} c_{k;n} x^k$, then

$$b_{l;n} = \delta_{l,n} = \frac{\sum_{k=0}^{n} c_{k;n} (x^k, \pi_l)}{(\pi_l, \pi_l)} = \frac{1}{(\pi_l, \pi_l)} \sum_{k=l}^{n} c_{k;n} (x^k, \pi_l)$$

In particular, the coefficient of the highest degree is the same, $b_{n;n} = 1$, such that

$$c_{n;n} = \frac{(\pi_n, \pi_n)}{(x^n, \pi_n)} \tag{10.5}$$

246. A first interesting consequence of **art.** 244 arises for the special class of polynomials $p_n(x) = x^n$. In that case, if $l > n$, then $(x^n, \pi_l) = 0$, but $(x^n, \pi_n) \ne 0$. Introducing (10.3) and using $(x^n, x^k) = (x^{n+k}, 1) = m_{n+k}$ yields, for $n \le l$,

$$(x^n, \pi_l) = \sum_{k=0}^{l} c_{k;l} m_{n+k}$$

which is written in matrix form, taking into account that $(x^n, \pi_l) = (x^n, \pi_n) \delta_{l,n}$ for $0 \le n \le l$, as

$$\begin{bmatrix} m_0 & m_1 & \cdots & m_l \\ m_1 & m_2 & \cdots & m_{l+1} \\ \vdots & \vdots & \vdots & \vdots \\ m_l & m_{l+1} & \cdots & m_{2l} \end{bmatrix} \begin{bmatrix} c_{0;l} \\ c_{1;l} \\ \vdots \\ c_{l;l} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ (x^l, \pi_l) \end{bmatrix}$$

The symmetric moment matrix

$$
M_l = \begin{bmatrix}
m_0 & m_1 & \cdots & m_l \\
m_1 & m_2 & \cdots & m_{l+1} \\
\vdots & \vdots & \vdots & \vdots \\
m_l & m_{l+1} & \cdots & m_{2l}
\end{bmatrix}
$$

is a $(l+1) \times (l+1)$ Hankel matrix[2]. The Gram Schmidt orthogonalization process
(**art.** 243) shows that there always exists an orthogonal set of polynomials, such that
a set of not all zero coefficients $\{c_{k;l}\}_{0 \le k \le l}$ exists. This implies that the determinant
of the left hand side moment matrix is non zero. By Cramer's rule (8.83), the
solution is

$$
c_{k;l} = \frac{\left(x^l, \pi_l\right) \mathrm{cofactor}_{l+1,k} M_l}{\det M_l}
$$

In particular,

$$
c_{l;l} = \frac{\det M_{l\ 1}}{\det M_l} \left(x^l, \pi_l\right) \tag{10.6}
$$

which is always different from zero.

For any polynomial $p_n(x) = \sum_{k=0}^n a_k x^k$, we can write, by applying (10.6) for
$n = l$,

$$
(p_n, \pi_n) = \sum_{k=0}^n a_k \left(x^k, \pi_n\right) = a_n \left(x^n, \pi_n\right) = a_n \frac{c_{n;n} \det M_n}{\det M_{n\ 1}}
$$

In particular, when choosing for $p_n(x) = \pi_n(x)$, we observe that

$$
\frac{\det M_n}{\det M_{n\ 1}} = \frac{(\pi_n, \pi_n)}{c_{n;n}^2} > 0 \tag{10.7}
$$

10.3 The three-term recursion

247. *The three term recursion.* As another, even more important application of
art. 244, we consider the polynomial $p_n(x) = x\pi_{n\ 1}(x)$, whose coefficients are

$$
b_{l;n} = \frac{(x\pi_{n\ 1}, \pi_l)}{(\pi_l, \pi_l)} = \frac{(\pi_{n\ 1}, x\pi_l)}{(\pi_l, \pi_l)} = \frac{(x\pi_l, \pi_{n\ 1})}{(\pi_l, \pi_l)}
$$

Since $x\pi_l$ is a polynomial of degree $l+1$, we know from **art.** 244 that $b_{l;n} = 0$ when
$n - 1 > l + 1$, thus when $l < n - 2$. Hence, we find that any set of orthogonal
polynomials possesses a three term recursion for $2 \le n \le l$

$$
x\pi_{n\ 1}(x) = b_{n;n}\pi_n(x) + b_{n\ 1;n}\pi_{n\ 1}(x) + b_{n\ 2;n}\pi_{n\ 2}(x) \tag{10.8}
$$

When $n = 1$, then $\pi_0(x)$ is a constant and $\pi_{1}(x) = 0$. Observe that any other

---

[2] We refer for properties of the Hankel matrix to Gantmacher (1959a, pp. 338-348).

polynomial $p_n(x) = x^j \pi_{n-j}(x)$ with $j > 1$, will result in a recursion with $2j+1$ terms because $\frac{(x^j \pi_{n-j}, \pi_l)}{(\pi_l, \pi_l)} = \frac{(x^j \pi_l, \pi_{n-j})}{(\pi_l, \pi_l)} = 0$ if $n - j > l + j$, thus $l < n - 2j$.

Further, taking the scalar product in (10.8) with x^{n-2} yields

$$\left(x\pi_{n-1}, x^{n-2}\right) = b_{n;n}\left(\pi_n, x^{n-2}\right) + b_{n-1;n}\left(\pi_{n-1}, x^{n-2}\right) + b_{n-2;n}\left(\pi_{n-2}, x^{n-2}\right)$$

Since $\left(x\pi_{n-1}, x^{n-2}\right) = \left(\pi_{n-1}, x^{n-1}\right)$ while $\left(\pi_j, x^{n-2}\right) = 0$ for $j > n - 2$, we find, beside $b_{n-2;n} = \frac{(\pi_{n-1}, x\pi_{n-2})}{(\pi_{n-2}, \pi_{n-2})}$, that

$$b_{n-2;n} = \frac{\left(\pi_{n-1}, x^{n-1}\right)}{\left(\pi_{n-2}, x^{n-2}\right)} = \frac{c_{n-1;n-1} \det M_{n-1} \det M_{n-3}}{c_{n-2;n-2} \left(\det M_{n-2}\right)^2} \tag{10.9}$$

where the last formula follows from (10.6). It demonstrates that $b_{n-2;n} \neq 0$. More over, (10.7) shows that for monic polynomials, i.e., if $c_{n;n} = 1$, that $b_{n-2;n} > 0$ and, thus, $(\pi_{n-1}(x), x\pi_{n-2}) > 0$. Substituting (10.3) in

$$b_{n-2;n} = \frac{(x\pi_{n-2}, \pi_{n-1})}{(\pi_{n-2}, \pi_{n-2})} = \frac{\sum_{k=1}^{n-1} c_{k-1;n-2}\left(x^k, \pi_{n-1}\right)}{(\pi_{n-2}, \pi_{n-2})} = \frac{c_{n-2;n-2}\left(x^{n-1}, \pi_{n-1}\right)}{(\pi_{n-2}, \pi_{n-2})}$$

leads with (10.5) to

$$b_{n-2;n} = \frac{c_{n-2;n-2}\left(\pi_{n-1}, \pi_{n-1}\right)}{c_{n-1;n-1}\left(\pi_{n-2}, \pi_{n-2}\right)} \tag{10.10}$$

Further,

$$b_{n-1;n} = \frac{(x\pi_{n-1}, \pi_{n-1})}{(\pi_{n-1}, \pi_{n-1})} = \frac{1}{(\pi_{n-1}, \pi_{n-1})} \int_a^b u\pi_{n-1}^2(u)\, dW(u) \tag{10.11}$$

shows that $b_{n-1;n}$ is positive if $b > a \geq 0$ and negative, if $b < a \leq 0$. It can only be zero provided symmetry holds, $a = -b$ and $w(u) = \frac{dW}{du} = w(-u)$.

The coefficient $b_{n;n}$ can be rewritten as

$$b_{n;n} = \frac{(x\pi_{n-1}(x), \pi_n)}{(\pi_n, \pi_n)} = \frac{\sum_{k=1}^{n} c_{k-1;n-1}\left(x^k, \pi_n\right)}{(\pi_n, \pi_n)} = \frac{c_{n-1;n-1}\left(x^n, \pi_n\right)}{(\pi_n, \pi_n)}$$

Using (10.5) leads to

$$b_{n;n} = \frac{c_{n-1;n-1}}{c_{n;n}} \tag{10.12}$$

The expressions (10.9) and (10.12) simplify for monic polynomials where $c_{n;n} = 1$.

248. Often, the three term recursion (10.8) is rewritten in normalized form with $\pi_n(x) = \widetilde{\pi}_n(x)\sqrt{(\pi_n, \pi_n)}$ as

$$\widetilde{\pi}_n(x) = (x - b_{n-1;n})\,\widetilde{\pi}_{n-1}(x)\frac{\sqrt{(\pi_{n-1}, \pi_{n-1})}}{b_{n;n}\sqrt{(\pi_n, \pi_n)}} - \widetilde{\pi}_{n-2}(x)\frac{b_{n-2;n}\sqrt{(\pi_{n-2}, \pi_{n-2})}}{b_{n;n}\sqrt{(\pi_n, \pi_n)}}$$

Substituting the expressions (10.12), (10.11) and (10.9) for the b coefficients yields

$$\widetilde{\pi}_n(x) = (x - b_{n-1;n})\,\widetilde{\pi}_{n-1}(x)\frac{\widetilde{c}_{n;n}}{\widetilde{c}_{n-1;n-1}} - \widetilde{\pi}_{n-2}(x)\frac{\widetilde{c}_{n;n}\widetilde{c}_{n-2;n-2}}{\widetilde{c}_{n-1;n-1}^2}$$

where $\widetilde{c}_{n;n} = \frac{c_{n;n}}{\sqrt{(\pi_n,\pi_n)}}$. Thus,

$$\widetilde{\pi}_n(x) = (A_n x + B_n)\,\widetilde{\pi}_{n-1}(x) - C_n\widetilde{\pi}_{n-2}(x) \tag{10.13}$$

where $A_n = \frac{\widetilde{c}_{n;n}}{\widetilde{c}_{n-1;n-1}}$, $B_n = -b_{n-1;n}\frac{\widetilde{c}_{n;n}}{\widetilde{c}_{n-1;n-1}}$ and $C_n = \frac{\widetilde{c}_{n;n}\widetilde{c}_{n-2;n-2}}{\widetilde{c}^2_{n-1;n-1}} = \frac{A_n}{A_{n-1}}$. The major advantage of the normalized expression is the relation $C_n = \frac{A_n}{A_{n-1}}$, as illustrated in **art.** 249.

The converse is proven by Favard: if a set of polynomials satisfies a three term recursion as (10.8), then the set of polynomials is orthogonal. Favard's theorem is proven in Chihara (1978, p. 22) for monic polynomials, where $A_n = 1$ and $C_n > 0$.

249. *Christoffel Darboux formula.* Multiplying both sides of the normalized three term recursion (10.13) by $\widetilde{\pi}_{n-1}(y)$,

$$\widetilde{\pi}_{n-1}(y)\,\widetilde{\pi}_n(x) = (A_n x + B_n)\,\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_{n-1}(y) - C_n\widetilde{\pi}_{n-2}(x)\,\widetilde{\pi}_{n-1}(y)$$

Similarly, letting $x \to y$ in (10.13) and multiplying both sides by $\widetilde{\pi}_{n-1}(x)$ yields

$$\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_n(y) = (A_n y + B_n)\,\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_{n-1}(y) - C_n\widetilde{\pi}_{n-2}(y)\,\widetilde{\pi}_{n-1}(x)$$

Subtracting the second equation from the first results in

$$\widetilde{\pi}_{n-1}(y)\,\widetilde{\pi}_n(x) - \widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_n(y) = A_n(x-y)\,\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_{n-1}(y)$$
$$- C_n\{\widetilde{\pi}_{n-2}(x)\,\widetilde{\pi}_{n-1}(y) - \widetilde{\pi}_{n-2}(y)\,\widetilde{\pi}_{n-1}(x)\}$$

At this stage, we employ the relation $C_n = \frac{A_n}{A_{n-1}}$, that only holds for the normalized three term recursion (10.13) and not for (10.8). Defining

$$g_n = \frac{\widetilde{\pi}_{n-1}(y)\,\widetilde{\pi}_n(x) - \widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_n(y)}{A_n}$$

leads to

$$(x-y)\,\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_{n-1}(y) = g_n - g_{n-1}$$

Summing both sides over n,

$$(x-y)\sum_{n=1}^{m+1}\widetilde{\pi}_{n-1}(x)\,\widetilde{\pi}_{n-1}(y) = \sum_{n=1}^{m+1} g_n - \sum_{n=1}^{m+1} g_{n-1}$$
$$= g_{m+1} - g_0 = g_{m+1}$$

because $\widetilde{\pi}_{-1} = 0$. Hence, we arrive at the famous Christoffel Darboux formula,

$$\sum_{n=0}^{m}\widetilde{\pi}_n(x)\,\widetilde{\pi}_n(y) = \frac{1}{A_{m+1}}\frac{\widetilde{\pi}_m(y)\,\widetilde{\pi}_{m+1}(x) - \widetilde{\pi}_m(x)\,\widetilde{\pi}_{m+1}(y)}{x-y} \tag{10.14}$$

which can also be written as

$$\sum_{n=0}^{m}\widetilde{\pi}_n(x)\,\widetilde{\pi}_n(y) = \frac{\widetilde{\pi}_m(y)\,\widetilde{\pi}_{m+1}(x) - \widetilde{\pi}_{m+1}(y)}{A_{m+1}}\frac{1}{x-y} - \frac{\widetilde{\pi}_{m+1}(y)\,\widetilde{\pi}_m(x) - \widetilde{\pi}_m(y)}{A_{m+1}}\frac{1}{x-y}$$

The special case, where $x = y$, follows, after invoking the definition of the derivative, as

$$\sum_{n=0}^{m} \widetilde{\pi}_n^2 (x) = \frac{\widetilde{\pi}_m (x) \widetilde{\pi}'_{m+1} (x) - \widetilde{\pi}'_m (x) \widetilde{\pi}_{m+1} (x)}{A_{m+1}} = \frac{\widetilde{\pi}_m^2 (x)}{A_{m+1}} \frac{d}{dx} \left(\frac{\widetilde{\pi}_{m+1} (x)}{\widetilde{\pi}_m (x)} \right)$$

(10.15)

250. *Associated orthogonal polynomials.* Similar to the derivation of the Christoffel Darboux formula in **art. 249**, we consider the difference at two arguments of the three term recursion (10.8) for $n > 1$,

$$x\pi_{n-1} (x) - y\pi_{n-1} (y) = b_{n;n} [\pi_n (x) - \pi_n (y)] + b_{n-1;n} [\pi_{n-1} (x) - \pi_{n-1} (y)]$$
$$+ b_{n-2;n} [\pi_{n-2} (x) - \pi_{n-2} (y)]$$

We rewrite the left hand side as

$$x\pi_{n-1} (x) - y\pi_{n-1} (y) = x [\pi_{n-1} (x) - \pi_{n-1} (y)] + (x - y) \pi_{n-1} (y)$$

and obtain

$$(x - y) \pi_{n-1} (y) = b_{n;n} [\pi_n (x) - \pi_n (y)] + (b_{n-1;n} - x) [\pi_{n-1} (x) - \pi_{n-1} (y)]$$
$$+ b_{n-2;n} [\pi_{n-2} (x) - \pi_{n-2} (y)]$$

After multiplying both sides by $\frac{dW(y)}{x-y}$ and integrating over $[a, b]$, we have

$$\int_a^b \pi_{n-1} (y) \, dW (y) = b_{n;n} \int_a^b \frac{\pi_n (x) - \pi_n (y)}{x - y} dW (y)$$
$$+ (b_{n-1;n} - x) \int_a^b \frac{\pi_{n-1} (x) - \pi_{n-1} (y)}{x - y} dW (y)$$
$$+ b_{n-2;n} \int_a^b \frac{\pi_{n-2} (x) - \pi_{n-2} (y)}{x - y} dW (y)$$

Since $\int_a^b \pi_{n-1} (y) \, dW (y) = (\pi_{n-1}, 1) = 0$ for $n > 1$ by orthogonality (**art. 244**), we arrive, with the definition

$$\sigma_n (x) = \int_a^b \frac{\pi_n (x) - \pi_n (y)}{x - y} dW (y)$$

(10.16)

at the same recursion as (10.8) for $n > 1$,

$$x\sigma_{n-1} (x) = b_{n;n}\sigma_n (x) + b_{n-1;n}\sigma_{n-1} (x) + b_{n-2;n}\sigma_{n-2} (x)$$

If $n = 0$, in which case $\pi_0 (x)$ is a constant, then (10.16) shows that $\sigma_0 (x) = 0$. For $n = 1$ where $\pi_1 (x) = c_{1;1}x + c_{0;1}$, the integral (10.16) with (10.4) gives $\sigma_1 (x) =$

$c_{1;1}m_0$. By introducing (10.3) in (10.16), we have

$$\sigma_n(x) = \sum_{k=0}^{n} c_{k;n} \int_a^b \frac{x^k - y^k}{x - y} dW(y)$$

$$= \sum_{k=0}^{n} c_{k;n} \sum_{j=0}^{k-1} x^j \int_a^b y^{k-1-j} dW(y)$$

Using (10.4) yields

$$\sigma_n(x) = \sum_{k=0}^{n} c_{k;n} \sum_{j=0}^{k-1} x^j m_{k-1-j}$$

After reversal of the summation, we find that

$$\sigma_n(x) = \sum_{j=0}^{n-1} \left(\sum_{k=j+1}^{n} c_{k;n} m_{k-1-j} \right) x^j$$

is a polynomial of order $n - 1$. Since the polynomials $\sigma_n(x)$ satisfy a three term recursion, Favard's theorem (**art. 247**) states that these polynomials are also orthogonal. The polynomials $\sigma_n(x)$, defined by the integral (10.16), are called *orthogonal polynomials of the second kind* or *associated orthogonal polynomials*. The analysis shows that, by choosing other initial conditions, another set of orthogonal polynomials can be obtained from the three term recursion (10.8).

251. The integral (10.16) of $\sigma_n(x)$ cannot be split into two integrals when $x \in [a, b]$, due to the pole at x. However, when $x \in \mathbb{C} \setminus [a, b]$, then we can write,

$$\sigma_n(x) = \pi_n(x) \int_a^b \frac{dW(y)}{x - y} - \int_a^b \frac{\pi_n(y)}{x - y} dW(y)$$

For $|x| > \max(|a|, |b|)$, we expand $\frac{1}{x-y} = \sum_{k=0}^{\infty} \frac{y^k}{x^{k+1}}$ and interchange the integration and summation (which is valid when assuming absolute convergence). The first integral,

$$F(x) = \int_a^b \frac{dW(y)}{x - y} \tag{10.17}$$

becomes

$$F(x) = \sum_{k=0}^{\infty} \frac{1}{x^{k+1}} \int_a^b y^k dW(y) = \sum_{k=0}^{\infty} \frac{m_k}{x^{k+1}}$$

while the second integral,

$$\rho_n(x) = \int_a^b \frac{\pi_n(y)}{x - y} dW(y) \tag{10.18}$$

reads

$$\rho_n(x) = \sum_{k=0}^{\infty} \frac{1}{x^{k+1}} \int_a^b y^k \pi_n(y) dW(y) = \sum_{k=n}^{\infty} \frac{(y^k, \pi_n)}{x^{k+1}}$$

because, by orthogonality (**art. 244**), $(y^k, \pi_n) = 0$ for $k < n$. Hence, for large x, we rewrite

$$\sigma_n(x) = \pi_n(x) F(x) - \rho_n(x)$$

as

$$\frac{\sigma_n(x)}{\pi_n(x)} = F(x) - \frac{\rho_n(x)}{\pi_n(x)} = F(x) + O\left(x^{-2n-1}\right) \tag{10.19}$$

whose consequences are further explored in **art.** 257. Convergence considerations when $n \to \infty$ are discussed in Gautschi (2004).

252. *Computing the weight function $w(x)$.* The two functions $F(z)$ and $\rho_n(z)$ are analytic in $\mathbb{C} \setminus [a, b]$ and both integral representations resemble the Cauchy integral, $f(z) = \frac{1}{2\pi i} \int_{C(z)} \frac{f(w)}{z-w} dw$, where $C(z)$ is a contour that encloses the point $z \in \mathbb{C}$. A general theorem (Markushevich, 1985, p. 312) states that the integral of the Cauchy type,

$$f(z) = \frac{1}{2\pi i} \int_L \frac{\varphi(w)}{z-w} dw$$

satisfies

$$\lim_{z \to z_0; z \in I(z_0)} f(z) - \lim_{w \to z_0; w \in E(z_0)} f(w) = \varphi(z_0)$$

where L is a (not necessarily closed) path in the complex plane and on which $|\varphi(z) - \varphi(z_0)| \leq c(z - z_0)^\beta$ for any point $z, z_0 \in L$, and where $c, \beta > 0$ are constants. The interior $I(z_0)$ is a region enclosed[3] by a closed contour $C(z_0)$ around $z_0 \in L$ in which $\varphi(w)$ is analytic. The exterior $E(z_0)$ is the region that is not enclosed by a contour $C'(z_0)$. The contours $C(z_0)$ and $C'(z_0)$ are here formed by a circle around z_0 with a radius such that it intersects the path L in two points z_1 and z_2 and such that $\varphi(w)$ is analytic in the enclosed region. The first contour $C(z_0)$ follows the path L in the positive direction from z_1 to z_2 and returns to z_1 along the circle in positive direction, whereas contour $C'(z_0)$ similarly follows the path L in the positive direction from z_1 to z_2, but it returns to z_1 along the circle around z_0 in negative direction. Hence, any point z lying inside the contour $C(z_0)$ is enclosed in positive direction, whereas any point w lying inside the contour $C'(z_0)$ is enclosed in negative direction. This direction does not contribute to the Cauchy integral, since it is equivalent to being not enclosed (see, e.g., Titchmarsh (1964)).

We apply this theorem to the integral (10.18). The path L is the segment $[a, b]$ on the real axis and $z_0 = x_0 \in [a, b]$. The contour $C(z_0)$ around $z_0 = x_0$ is the path from $x_0 - r > a$ to $x_0 + r < b$ along the real axis and the circle segment lying above the real axis (with positive imaginary part). The contour $C'(z_0)$ follows the same

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[3] An observer traveling in the direction of the contour around z_0 finds the interior on his left and the exterior on his right.

segment from $x_0 - r > a$ to $x_0 + r < b$, but returns along the semicircle below the real axis. Hence,

$$\lim_{z \to z_0; z \in I(z_0)} \rho_n(z) = \lim_{y \to 0} \rho_n(x_0 + iy)$$

$$\lim_{w \to z_0; w \in E(z_0)} \rho_n(w) = \lim_{y \to 0} \rho_n(x_0 - iy)$$

Since the complex conjugate $\rho_n^*(z) = \rho_n(z^*)$, by the reflection principle (Titchmarsh, 1964, p. 155) because $\rho_n(z)$ is real on the real axis, we have that

$$\rho_n(x_0 - iy) = \operatorname{Re}\rho_n(x_0 - iy) + i\operatorname{Im}\rho_n(x_0 - iy)$$
$$= \operatorname{Re}\rho_n(x_0 + iy) - i\operatorname{Im}\rho_n(x_0 + iy)$$

and, finally,

$$\frac{1}{\pi} \lim_{y \to 0} \operatorname{Im}\rho_n(x_0 + iy) = \pi_n(x_0) w(x_0)$$

Similarly, from the integral (10.17), the density function is found at $x_0 \in [a, b]$ by

$$w(x_0) = \frac{1}{\pi} \lim_{y \to 0} \operatorname{Im} F(x_0 + iy)$$

10.4 Zeros of orthogonal polynomials

As will be illustrated, a lot of information about the zeros of orthogonal polynomials can be deduced. We remark that $\pi_n(x) = \widetilde{\pi}_n(x) \sqrt{(\pi_n, \pi_n)}$ shows that both the orthogonal polynomial and its normalized version possess the same zeros.

253. *Zeros of orthogonal polynomials.*

Theorem 66 *All zeros of the orthogonal polynomial $\pi_l(u)$ are real, simple and lie inside the interval $[a, b]$.*

Proof: Art. 246 has shown that $(x^n, \pi_l) = 0$ if $n < l$. The particular case $n = 0$ and $l \geq 1$, written with (10.1) as

$$\int_a^b \pi_l(u) \, dW(u) = 0$$

indicates that there must exist at least one point within the interval (a, b) at which $\pi_l(u)$ changes sign because $W(u)$ is a distribution function with positive density. The change in sign implies that such a point is a zero with odd multiplicity. Let $z_1, z_2, \ldots, z_k$ be all such points and consider the polynomial $q_k(x) = \prod_{j=1}^{k}(x - z_j)$. **Art.** 244 shows that $(\pi_l, q_l) \neq 0$ but that $(\pi_l, q_k) = 0$ if $l > k$,

$$\int_a^b \pi_l(u) \prod_{j=1}^{k}(x - z_j) \, dW(u) = 0$$

By construction, $\pi_l(u) \prod_{j=1}^{k} (x - z_j)$ does not change sign for any $x \in [a, b]$ and, hence, the integral cannot vanish. Orthogonality shows that the non vanishing of (π_l, q_k) is only possible provided $k = l$. The fundamental theorem of algebra (**art.** 196) together with the odd multiplicity of each zero z_j then implies that all zeros are simple. $\square$

Szegő (1978, p. 45) presents other proofs. For example, the simplicity of the zeros can be deduced by applying the Sturm sequence (**art.** 224) to the tree term recursion (10.13) (assuming $c_{n;n} > 0$). Theorem 66 shows that any orthogonal polynomial only possesses real and simple zeros. An arbitrary polynomial with real coefficients possesses zeros that, with high probability, do not all lie on a line segment in the complex plane, which illustrates the peculiar nature of orthogonal polynomials.

Let $a \le z_{n;n} < z_{n-1;n} < \cdots < z_{1;n} \le b$ denote the zeros of the orthogonal polynomial $\pi_n(x)$. Combining Theorem 66 and (9.1) yields

$$\pi_n(x) = c_{n;n} \prod_{j=1}^{n} (x - z_{j;n}) \tag{10.20}$$

254. *Interlacing property of zeros of orthogonal polynomials.* The main observations are derived from the Christoffel Darboux formula (10.15), which implies, assuming $A_{n+1} > 0$,

$$\widetilde{\pi}_n(x) \widetilde{\pi}'_{n+1}(x) - \widetilde{\pi}'_n(x) \widetilde{\pi}_{n+1}(x) \ge \frac{1}{m_0} > 0 \tag{10.21}$$

because $\widetilde{\pi}_0(x) = \frac{1}{\sqrt{m_0}}$. The simplicity of the zeros (Theorem 66) implies that the derivative $\widetilde{\pi}'_m(x)$ cannot have the same zero as $\widetilde{\pi}_m(x)$. Hence, the above inequality indicates that $\widetilde{\pi}_m(x)$ and $\widetilde{\pi}_{m+1}(x)$ cannot have a same zero.

Theorem 67 (Interlacing) *Let $a < z_{n;n} < z_{n-1;n} < \cdots < z_{1;n} < b$ be the zeros of the orthogonal polynomial $\pi_n(x)$. The zeros of $\pi_n(x)$ and $\pi_{n+1}(x)$ are interlaced,*

$$a < z_{n+1;n+1} < z_{n;n} < z_{n;n+1} < z_{n-1;n} < \cdots < z_{1;n} < z_{1;n+1} < b$$

In other words, between each pair of consecutive zeros of $\pi_n(x)$, there lies a zero of $\pi_{n+1}(x)$, thus, $z_{k;n} < z_{k;n+1} < z_{k-1;n}$ for all $1 \le k \le n$, while the smallest and largest zero obey $a < z_{n+1;n+1} < z_{n;n}$ and $z_{1;n} < z_{1;n+1} < b$.

Proof: Theorem 66 shows that the zeros are simple and real such that

$$\pi'_n(z_{k;n}) \pi'_n(z_{k-1;n}) < 0$$

On the other hand, the inequality (10.21) implies that

$$-\pi'_n(z_{k;n}) \pi_{n+1}(z_{k;n}) > 0 \quad \text{and} \quad -\pi'_n(z_{k-1;n}) \pi_{n+1}(z_{k-1;n}) > 0$$

Multiplying both and taking $\pi'_n(z_{k;n}) \pi'_n(z_{k-1;n}) < 0$ into account yields

$$\pi_{n+1}(z_{k;n}) \pi_{n+1}(z_{k-1;n}) < 0$$

which means that there is at least one zero $z_{j;n+1}$ between $z_{k;n} < z_{j;n+1} < z_{k-1;n}$. Since the inequalities hold for all $1 \leq k \leq n$, the argument accounts for at least $n-1$ zeros of $\pi_{n+1}(x)$. With the convention that $c_{n;n} > 0$ for all $n \geq 0$, we know that $\pi_n(x)$ is increasing at least from the largest zero on, $\pi'_n(z_{1;n}) > 0$. The inequality (10.21) indicates that $\pi_{n+1}(z_{1;n}) < 0$. By the convention $c_{n;n} > 0$ for all $n \geq 0$, we have that $\pi_{n+1}(b) > 0$ such that there must be a zero, in fact the largest $z_{1;n+1}$ of $\pi_{n+1}(x)$ in the interval $[z_{1;n}, b]$. A similar argument applies for the smallest zero $z_{n+1;n+1}$, thereby proving the theorem. $\qquad \square$

If $z_{n;n} = a$, the interlacing Theorem 67 implies that the set $\{\widetilde{\pi}_k(x)\}_{0 \leq k \leq n}$ is finite and that $\widetilde{\pi}_n(x)$ is the highest order polynomial of that finite orthogonal set with a zero equal to $z_{n;n} = a$. All other smallest zeros are larger, i.e., $z_{k;k} > a$ for $1 \leq k \leq n-1$.

Another noteworthy consequence of the interlacing Theorem 67 is the partial fraction decomposition

$$\frac{\pi_n(x)}{\pi_{n+1}(x)} = \sum_{k=1}^{n+1} \frac{\beta_{k;n+1}}{x - z_{k;n+1}}$$

where the coefficients, in general, obey

$$\beta_{k;n+1} = \lim_{x \to z_{k;n+1}} \frac{\pi_n(x)(x - z_{k;n+1})}{\pi_{n+1}(x)} = \frac{\pi_n(z_{k;n+1})}{\pi'_{n+1}(z_{k;n+1})}$$

Inequality (10.21) shows that all $\beta_{k;n+1} > 0$. We include here a sharpening of the interlacing property whose proof relies on the Gaussian quadrature Theorem 69 derived in Section 10.5.

Theorem 68 *Between two zeros of $\pi_n(x)$, there is at least one zero of $\pi_l(x)$ with $l > n$.*

Proof: Assume the contrary, namely $\pi_l(x)$ has no zero between $z_{k;n}$ and $z_{k-1;n}$ for some $k \in [1, n]$. Then, the polynomial $p_m(x) = \pi_n(x) q_{n-2}(x)$ of degree $m = 2n-2$, where

$$q_{n-2}(x) = \frac{\pi_n(x)}{(x - z_{k;n})(x - z_{k-1;n})}$$

is everywhere non zero in $[a, b]$, except in the interval $(z_{k;n}, z_{k-1;n})$, where $p_m(x)$ is negative. The Gaussian quadrature Theorem 69 shows, for $m = 2n - 2 < 2l$, that

$$\int_a^b p_m(x)\, dW(x) = \sum_{j=1}^l p_m(z_{j;l}) \lambda_{j;l} > 0$$

because (a) the Christoffel numbers $\lambda_{j;l}$ are positive (**art. 256**), and (b) $p_m(z_{j;l})$ cannot vanish at every zero $z_{j;l}$ of $\pi_l(x)$ and $p_m(z_{j;l}) \geq 0$ since, by hypothesis,

$z_{j;l} \notin [z_{k;n}, z_{k\ 1;n}]$. But this contradicts the basic orthogonality property,

$$\int_a^b p_m(x)\, dW(x) = (\pi_n, q_{n\ 2}) = 0$$

established in **art. 244**.   □

Szegő (1978, p. 112) mentions the following distance result between consecutive zeros. If the density or weight function $\frac{dW(x)}{dx} = w(x) \geq w_{\min} > 0$ and the zeros are written as $z_{k;n} = \frac{a+b}{2} + \frac{b\ a}{2}\cos\theta_{k;n}$, where $0 < \theta_{k;n} < \pi$, for $1 \leq k \leq n$, then it holds that

$$\theta_{k+1;n} - \theta_{k;n} < \alpha \frac{\log n}{n}$$

where the constant α depends on $w_{\min}$, a and b. If stronger constraints are imposed on the weight function w, the $\log n$ factor in the numerator can be removed. More precise results on the location of zeros only seem possible in specific cases and/or when the differential equation of the set of orthogonal polynomials is known.

10.5 Gaussian quadrature

Lanczos (1988, pp. 396 414) nicely explains Gauss's genial idea to compute the integral $\int_{\ 1}^1 f(u)\, du$ with "double order accuracy" compared to other numerical integration methods. The underlying principle of Gauss's renowned quadrature method is orthogonality and properties of orthogonal polynomials. Before giving an example, we first focus on the theory.

255. We consider the Lagrange polynomial $q_{n\ 1}$ of degree $n-1$ (**art. 206**) that coincides at n points, defined by their finite coordinates (x_j, y_j) for $1 \leq j \leq n$, with the arbitrary polynomial $p_m(x)$ of degree $m > n$,

$$q_{n\ 1}(x) = \sum_{j=1}^n y_j l_{n\ 1}(x; x_k) = \sum_{j=1}^n y_j \frac{F_n(x)}{(x - x_j) F_n'(x_j)}$$

where $F_n(x) = \prod_{j=1}^n (x - x_j)$ and $y_j = p_m(x_j)$. We further assume that the abscissa coincide with the (distinct) zeros of the orthogonal polynomial $\pi_n(x)$, thus $x_j = z_{j;n}$. Then, from (10.20), it follows that $\frac{F_n(x)}{F_n'(z_{j;n})} = \frac{\pi_n(x)}{\pi_n'(z_{j;n})}$ for all $1 \leq j \leq n$ and we obtain

$$q_{n\ 1}(x) = \sum_{j=1}^n p_m(z_{j;n}) \frac{\pi_n(x)}{(x - z_{j;n}) \pi_n'(z_{j;n})}$$

Moreover, the difference polynomial $r_m(x) = p_m(x) - q_{n\ 1}(x)$ has degree m and $r_m(x)$ vanishes at the n points $x_j = z_{j;n}$, taken as the zeros of $\pi_n(x)$. Thus,

$$r_m(x) = t_{m\ n}(x) \pi_n(x)$$

where $t_{m\ n}(x)$ is some polynomial of degree $m - n$. Taking the scalar product $(r_m, 1)$ (or multiplying both sides by $dW(x)$ and integrating over $[a, b]$) shows that

$$(r_m, 1) = (t_{m\ n}, \pi_n)$$

which, by **art. 244**, vanishes provided $n > m - n$, or $2n > m$. In the case that m is at most $2n - 1$ and $(r_m, 1) = (p_m - q_{n\ 1}, 1) = 0$, we find that

$$\int_a^b p_m(x)\, dW(x) = \int_a^b q_{n\ 1}(x)\, dW(x)$$
$$= \sum_{j=1}^n p_m(z_{j;n}) \int_a^b \frac{\pi_n(x)\, dW(x)}{(x - z_{j;n})\, \pi_n'(z_{j;n})}$$

In summary, we have demonstrated Gauss's famous quadrature formula,

Theorem 69 (Gauss's quadrature formula) *Let* $a < z_{n;n} < z_{n\ 1;n} < \cdots < z_{1;n} < b$ *be the zeros of the orthogonal polynomial* $\pi_n(x)$. *For any polynomial* $p_m(x)$ *of degree* m *at most* $2n - 1$,

$$\int_a^b p_m(x)\, dW(x) = \sum_{j=1}^n p_m(z_{j;n})\, \lambda_{j;n} \tag{10.22}$$

where the Christoffel numbers are

$$\lambda_{j;n} = \int_a^b \frac{\pi_n(x)\, dW(x)}{(x - z_{j;n})\, \pi_n'(z_{j;n})} \tag{10.23}$$

and $\pi_n(x)$ *is orthogonal on the interval* $[a, b]$ *with respect to the distribution function* $W(x)$.

256. The Christoffel numbers possess interesting properties. First, let $p_m(x) = \left\{ \frac{\pi_n(x)}{(x\ z_{j;n})\pi_n'(z_{j;n})} \right\}^2$ such that $p_m(z_{k;n}) = \delta_{kj}$, then Gauss's quadrature formula (10.22) reduces to

$$\lambda_{j;n} = \int_a^b \left\{ \frac{\pi_n(x)}{(x - z_{j;n})\, \pi_n'(z_{j;n})} \right\}^2 dW(x) \tag{10.24}$$

demonstrating that all Christoffel numbers $\lambda_{j;n}$ are positive.

The integral (10.18), corresponding to the associated orthogonal polynomials $\sigma_n(x)$ and valid for $x \in \mathbb{C} \setminus [a, b]$, actually is finite at the zeros of $\pi_n(x)$. Comparison with (10.23) shows that

$$\rho_n(z_{j;n}) = -\lambda_{j;n} \pi_n'(z_{j;n})$$

Next, the Christoffel Darboux formula (10.14), with $y = z_{j;n}$, is

$$\sum_{k=0}^{n\ 1} \widetilde{\pi}_k(x)\, \widetilde{\pi}_k(z_{j;n}) = \frac{1}{A_{n+1}} \frac{-\widetilde{\pi}_n(x)\, \widetilde{\pi}_{n+1}(z_{j;n})}{x - z_{j;n}}$$

Taking the scalar product $(.,1)$ of both sides yields

$$\sum_{k=0}^{n\ 1} (\widetilde{\pi}_k, 1)\, \widetilde{\pi}_k (z_{j;n}) = -\frac{\widetilde{\pi}_{n+1}(z_{j;n})}{A_{n+1}} \int_a^b \frac{\widetilde{\pi}_n(x)}{x - z_{j;n}} dW(x)$$

Art. 244 shows that $(\widetilde{\pi}_k, 1) = 0$ except when $k = 0$. In that case, $\widetilde{\pi}_0(x) = \frac{1}{\sqrt{m_0}}$ and $(\widetilde{\pi}_0, 1) = \int_a^b \widetilde{\pi}_0(x)\, dW(x) = \sqrt{m_0}$ such that

$$\sum_{k=0}^{n\ 1} (\widetilde{\pi}_k, 1)\, \widetilde{\pi}_k (z_{j;n}) = 1$$

The definition (10.23) of the Christoffel numbers shows that

$$\lambda_{j;n} = \int_a^b \frac{\pi_n(x)\, dW(x)}{(x - z_{j;n})\, \pi_n'(z_{j;n})} = \int_a^b \frac{\widetilde{\pi}_n(x)\, dW(x)}{(x - z_{j;n})\, \widetilde{\pi}_n'(z_{j;n})}$$

such that

$$1 = -\frac{\widetilde{\pi}_{n+1}(z_{j;n})}{A_{n+1}} \int_a^b \frac{\widetilde{\pi}_n(x)}{x - z_{j;n}} dW(x) = -\frac{\widetilde{\pi}_{n+1}(z_{j;n})\, \widetilde{\pi}_n'(z_{j;n})}{A_{n+1}} \lambda_{j;n}$$

Thus, the Christoffel numbers obey

$$\lambda_{j;n} = -\frac{A_{n+1}}{\widetilde{\pi}_{n+1}(z_{j;n})\, \widetilde{\pi}_n'(z_{j;n})} = \frac{A_n}{\widetilde{\pi}_{n\ 1}(z_{j;n})\, \widetilde{\pi}_n'(z_{j;n})} \tag{10.25}$$

where the latter follows from (10.13).

Finally, the Christoffel Darboux formula (10.15) evaluated at $x = z_{j;n}$ combined with (10.25) gives

$$\lambda_{j;n} = \frac{1}{\sum_{k=0}^{n\ 1} \widetilde{\pi}_k^2(z_{j;n})} \tag{10.26}$$

257. *Partial fraction decomposition of* $\frac{\sigma_n(x)}{\pi_n(x)}$. The associated orthogonal polyno mials (**art.** 250) are of degree $n - 1$, such that the fraction $\frac{\sigma_n(x)}{\pi_n(x)}$ can be expanded as

$$\frac{\sigma_n(x)}{\pi_n(x)} = \sum_{k=1}^{n} \frac{a_{k;n}}{x - z_{k;n}}$$

where we need to determine the coefficients $a_{k;n}$. Equation (10.19) shows that, for large x,

$$\frac{\sigma_n(x)}{\pi_n(x)} - F(x) = O\left(x^{\ 2n\ 1}\right)$$

With the integral (10.17) of $F(x)$, we have

$$\sum_{k=1}^{n} \frac{a_{k;n}}{x - z_{k;n}} - \int_a^b \frac{dW(y)}{x - y} = O\left(x^{\ 2n\ 1}\right)$$

After expanding the left hand side in a power series in x^{-1} and after equating the corresponding power of x^{-m}, we obtain, for $0 \leq m \leq 2n - 1$,

$$\sum_{k=1}^{n} a_{k;n} \left(z_{k;n} \right)^m - \int_a^b y^m dW \left(y \right) = 0$$

Gauss's quadrature formula (10.22) applied to $p_m \left(x \right) = y^m$ for $0 \leq m \leq 2n - 1$ gives

$$\int_a^b y^m dW \left(y \right) = \sum_{k=1}^{n} \lambda_{k;n} z_{k;n}^m$$

whence $a_{k;n} = \lambda_{k;n}$. In summary, the partial fraction decomposition becomes

$$\frac{\sigma_n \left(x \right)}{\pi_n \left(x \right)} = \sum_{k=1}^{n} \frac{\lambda_{k;n}}{x - z_{k;n}}$$

from which the Christoffel numbers follow as

$$\lambda_{j;n} = \lim_{x \to z_{j;n}} \frac{\sigma_n \left(x \right) \left(x - z_{j;n} \right)}{\pi_n \left(x \right)} = \frac{\sigma_n \left(z_{j;n} \right)}{\pi_n' \left(z_{j;n} \right)} \tag{10.27}$$

258. *Parameterized weight functions.* Suppose that the distribution function W is differentiable at any point of $[a, b]$, and that W depends on a parameter t. In addition, we assume that the density or weight function $w \left(x, t \right) = \frac{dW \left(x, t \right)}{dx}$ is positive and that $w \left(x, t \right)$ is also continuous and differentiable in t. The explicit dependence on the parameter t in Gauss's quadrature formula (10.22) is written as

$$\int_a^b p_m \left(x \right) w \left(x, t \right) dx = \sum_{j=1}^{n} p_m \left(z_{j;n} \left(t \right) \right) \lambda_{j;n} \left(t \right)$$

Differentiation with respect to t yields

$$\int_a^b p_m \left(x \right) \frac{\partial w \left(x, t \right)}{\partial t} dx = \sum_{j=1}^{n} p_m' \left(z_{j;n} \left(t \right) \right) z_{j;n}' \left(t \right) \lambda_{j;n} \left(t \right) + \sum_{j=1}^{n} p_m \left(z_{j;n} \left(t \right) \right) \lambda_{j;n}' \left(t \right)$$

For the particular choice of $p_m \left(x \right) = \frac{\widetilde{\pi}_n^2 \left(x, t \right)}{x - z_{k;n} \left(t \right)}$, we have that $p_m \left(z_{j;n} \left(t \right) \right) = 0$ and that

$$p_m' \left(z_{j;n} \left(t \right) \right) = \left. \frac{dp_m \left(x \right)}{dx} \right|_{x = z_{j;n} \left(t \right)} = \left(\widetilde{\pi}_n' \left(z_{j;n} \left(t \right), t \right) \right)^2 \delta_{jk}$$

such that

$$\int_a^b \frac{\widetilde{\pi}_n^2 \left(x, t \right)}{x - z_{k;n} \left(t \right)} \frac{\partial w \left(x, t \right)}{\partial t} dx = \left(\widetilde{\pi}_n' \left(z_{k;n} \left(t \right), t \right) \right)^2 z_{k;n}' \left(t \right) \lambda_{k;n} \left(t \right)$$

On the other hand,

$$\left(\widetilde{\pi}_n, \frac{\widetilde{\pi}_n}{x - z_{k;n} \left(t \right)} \right) = \int_a^b \frac{\widetilde{\pi}_n^2 \left(x, t \right)}{x - z_{k;n} \left(t \right)} w \left(x, t \right) dx = 0$$

by orthogonality (**art.** 244). Subtraction from the previous integral yields

$$\left(\widetilde{\pi}_n'\left(z_{k;n}\left(t\right),t\right)\right)^2 z_{k;n}'\left(t\right)\lambda_{k;n}\left(t\right) = \int_a^b \frac{\widetilde{\pi}_n^2\left(x,t\right)}{x - z_{k;n}\left(t\right)}\left\{\frac{\partial w\left(x,t\right)}{\partial t} - \xi w\left(x,t\right)\right\}dx$$

$$= \int_a^b \frac{\widetilde{\pi}_n^2\left(x,t\right)}{x - z_{k;n}\left(t\right)}\left\{\frac{\frac{\partial w(x,t)}{\partial t}}{w\left(x,t\right)} - \xi\right\}w\left(x,t\right)dx$$

where, if the constant ξ is chosen equal to $\xi = \left.\frac{1}{w(x,t)}\frac{\partial w(x,t)}{\partial t}\right|_{x=z_{k;n}(t)}$ shows that the function

$$\frac{\left\{\frac{1}{w(x,t)}\frac{\partial w(x,t)}{\partial t} - \left.\frac{1}{w(x,t)}\frac{\partial w(x,t)}{\partial t}\right|_{x=z_{k;n}(t)}\right\}}{x - z_{k;n}\left(t\right)} \geq 0$$

provided that $\frac{1}{w(x,t)}\frac{\partial w(x,t)}{\partial t}$ is increasing in x. In that case, the integral at the right hand side is positive (because it cannot vanish at any point $x \in [a,b]$) and, hence, $z_{k;n}'\left(t\right) > 0$: the zero $z_{k;n}\left(t\right)$ of $\widetilde{\pi}_n\left(x,t\right)$ is increasing in the parameter t.

An interesting application is the choice $w\left(x,t\right) = \left(1-t\right)w_1\left(x\right) + tw_2\left(x\right)$, where w_1 and w_2 are two weight functions on $[a,b]$, both positive and continuous for $x \in \left(a,b\right)$. In addition,

$$\frac{1}{w\left(x,t\right)}\frac{\partial w\left(x,t\right)}{\partial t} = \frac{w_2\left(x\right) - w_1\left(x\right)}{\left(1-t\right)w_1\left(x\right) + tw_2\left(x\right)}$$

$$= \frac{1}{t}\left(1 - \frac{1}{t\frac{w_2(x)}{w_1(x)} + 1 - t}\right)$$

is increasing if $\frac{w_2(x)}{w_1(x)}$ is increasing for $0 < t < 1$. Then, we have shown above that the zero $z_{k;n}\left(t\right)$ of $\widetilde{\pi}_n\left(x,t\right)$ is increasing in t. Let $\{z_{1;k;n}\}_{1\leq k\leq n}$ and $\{z_{2;k;n}\}_{1\leq k\leq n}$ denote the set of zeros of the orthogonal polynomials corresponding to w_1 and w_2, respectively. Thus, $z_{2;k;n} = z_{k;n}\left(1\right)$ is larger than $z_{1;k;n} = z_{k,n}\left(0\right)$ for all $1 \leq k \leq n$, because $w\left(x,0\right) = w_1\left(x\right)$ and $w\left(x,1\right) = w_2\left(x\right)$. In summary, if the ratio $\frac{w_2(x)}{w_1(x)}$ of two weight functions is increasing on $x \in [a,b]$, then the respective zeros obey $z_{2;k;n} > z_{1;k;n}$ for all $1 \leq k \leq n$.

259. *Numerical integration.* Let us consider the integral

$$\int_a^b f\left(x\right)dW\left(x\right)$$

which exists for the function $f\left(x\right)$. The Gaussian quadrature formula (10.22) suggests

$$\int_a^b f\left(x\right)dW\left(x\right) = \sum_{j=1}^n f\left(z_{j;n}\right)\lambda_{j;n} + R_m$$

where the n term sum approximates the integral and where R_m represents the error. The Christoffel numbers $\{\lambda_{j;n}\}_{1\leq j\leq n}$ and the zeros $\{z_{j;n}\}_{1\leq j\leq n}$ of the orthogonal

polynomial $\pi_n (x)$ are independent of the function $f (x)$. Theorem 69 states that the above approximation is exact for any polynomial $f (x)$ of degree at most $2n - 1$. In fact, it can be shown (see Gautschi (2004)) that the Gaussian quadrature formula is the only interpolating quadrature rule with the largest possible precision of $2n - 1$.

Since $dW (u) = du$ for Legendre polynomials $P_n (x)$, where $a = -1$ and $b = 1$, the most straightforward numerical computation of the integral $\int_a^b f (u)\, du$ uses Legendre's orthogonal polynomials. After substitution $u = \frac{b+a}{2} + \frac{b-a}{2}x$, we have

$$\int_a^b f (u)\, du = \frac{b - a}{2} \int_1^1 f \left(\frac{b + a}{2} + \frac{b - a}{2}x \right) dx$$

We refer to Lanczos (1988, p. 400 404) for a numerical example that illustrates the power of the Gaussian quadrature formula.

10.6 The Jacobi matrix

260. *The Jacobi matrix.* The three term recursion (10.8) is written in matrix form by defining the vector $\tau (x) = \begin{bmatrix} \pi_0 (x) & \pi_1 (x) & \cdots & \pi_{n-1} (x) \end{bmatrix}^T$ as

$$
x
\begin{bmatrix}
\pi_0 (x) \\
\pi_1 (x) \\
\vdots \\
\pi_{n-2}(x) \\
\pi_{n-1}(x)
\end{bmatrix}
=
\begin{bmatrix}
b_{0;1} & b_{1;1} & & & \\
b_{0;2} & b_{1;2} & b_{2;2} & & \\
& \ddots & \ddots & \ddots & \\
& & b_{n-3;n-1} & b_{n-2;n-1} & b_{n-1;n-1} \\
& & & b_{n-2;n} & b_{n-1;n}
\end{bmatrix}
\begin{bmatrix}
\pi_0 (x) \\
\pi_1 (x) \\
\vdots \\
\pi_{n-2}(x) \\
\pi_{n-1}(x)
\end{bmatrix}
+
\begin{bmatrix}
0 \\
0 \\
\vdots \\
0 \\
b_n\pi_n(x)
\end{bmatrix}
$$

Thus,

$$x\tau (x) = \Upsilon\tau (x) + b_n\pi_n (x)\, e_n \tag{10.28}$$

where the basic vector $e_n = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \end{bmatrix}^T$ and the $n \times n$ matrix

$$
\Upsilon =
\begin{bmatrix}
b_{0;1} & b_{1;1} & & & \\
b_{0;2} & b_{1;2} & b_{2;2} & & \\
& \ddots & \ddots & \ddots & \\
& & b_{n-3;n-1} & b_{n-2;n-1} & b_{n-1;n-1} \\
& & & b_{n-2;n} & b_{n-1;n}
\end{bmatrix}
$$

We observe that, when $x = z_k$ is a zero of $\pi_n (x)$, then (10.28) reduces to the eigenvalue equation

$$\Upsilon\tau (z_k) = z_k\tau (z_k)$$

such that the zero z_k is an eigenvalue of Υ belonging to the eigenvector $\tau (z_k)$. This eigenvector is never equal to the zero vector because the first component $\pi_0 (x) = c_{0;0} \neq 0$.

There must be a similarity transform to make the matrix Υ symmetric, since all

zeros of $\pi_n(x)$ are real (Theorem 66). A similarity transform (**art.** 142) preserves the eigenvalues. The simplest similarity transform is $H = \mathrm{diag}(h_1, h_2, \ldots, h_n)$ such that

$$
\widetilde{\Upsilon} = H\Upsilon H^{-1} = \begin{bmatrix}
b_{0;1} & \frac{h_1}{h_2}b_{1;1} & & & & \\
\frac{h_2}{h_1}b_{0;2} & b_{1;2} & \frac{h_2}{h_3}b_{2;2} & & & \\
& \ddots & & \ddots & & \ddots \\
& & \frac{h_{n-1}}{h_{n-2}}b_{n-3;n-1} & b_{n-2;n-1} & \frac{h_{n-1}}{h_n}b_{n-1;n-1} \\
& & & \frac{h_n}{h_{n-1}}b_{n-2;n} & b_{n-1;n}
\end{bmatrix}
$$

Thus, in order to produce a symmetric matrix $\widetilde{\Upsilon} = \widetilde{\Upsilon}^T$, we need to require that $\left(\widetilde{\Upsilon}\right)_{i,i-1} = \left(\widetilde{\Upsilon}\right)_{i-1,i}$ for all $1 \leq i \leq n$, implying that, for $i \geq 2$,

$$
\frac{h_i}{h_{i-1}}b_{i-2;i} = \frac{h_{i-1}}{h_i}b_{i-1;i-1}
$$

whence

$$
\left(\frac{h_i}{h_{i-1}}\right)^2 = \frac{b_{i-1;i-1}}{b_{i-2;i}}
$$

Art. 247 shows that $b_{i-1;i-1}$ and $b_{i-2;i}$ have the same sign. Thus, $h_i = \sqrt{\frac{b_{i-1;i-1}}{b_{i-2;i}}}h_{i-1}$ for $1 \leq i \leq n$ and we can choose $h_1 = 1$ such that

$$
h_i = \sqrt{\prod_{k=1}^{j-1} \frac{b_{k;k}}{b_{k-1;k+1}}}
$$

The eigenvector belonging to zero z_k equals $\widetilde{\tau}(z_k) = H\tau(z_k)$. After the similarity transform H, the result for $\widetilde{\Upsilon}$ is the matrix

$$
\begin{bmatrix}
b_{0;1} & \sqrt{b_{0;2}b_{1;1}} & & & & \\
\sqrt{b_{0;2}b_{1;1}} & b_{1;2} & \sqrt{b_{1;3}b_{2;2}} & & & \\
& \ddots & & \ddots & & \ddots \\
& & \sqrt{b_{n-3;n-1}b_{n-2;n-2}} & b_{n-2;n-1} & \sqrt{b_{n-2;n}b_{n-1;n-1}} \\
& & & \sqrt{b_{n-2;n}b_{n-1;n-1}} & b_{n-1;n}
\end{bmatrix}
$$

261. Similarly as in **art.** 260, the three term recursion (10.13) of the normalized polynomials $\{\widetilde{\pi}_j(x)\}_{0 \leq j \leq n-1}$ is written in matrix form as

$$
x\begin{bmatrix}
\widetilde{\pi}_0(x) \\
\widetilde{\pi}_1(x) \\
\vdots \\
\widetilde{\pi}_{n-2}(x) \\
\widetilde{\pi}_{n-1}(x)
\end{bmatrix} = \begin{bmatrix}
-\frac{B_1}{A_1} & \frac{1}{A_1} & & & \\
\frac{1}{A_1} & -\frac{B_2}{A_2} & \frac{1}{A_2} & & \\
& \ddots & \ddots & \ddots & \\
& & \frac{1}{A_{n-2}} & -\frac{B_{n-1}}{A_{n-1}} & \frac{1}{A_{n-1}} \\
& & & \frac{1}{A_{n-1}} & -\frac{B_n}{A_n}
\end{bmatrix}\begin{bmatrix}
\widetilde{\pi}_0(x) \\
\widetilde{\pi}_1(x) \\
\vdots \\
\widetilde{\pi}_{n-2}(x) \\
\widetilde{\pi}_{n-1}(x)
\end{bmatrix} + \begin{bmatrix}
0 \\
0 \\
\vdots \\
0 \\
\frac{1}{A_n}\widetilde{\pi}_n(x)
\end{bmatrix}
$$

Thus, in the normalized case where $C_n = \frac{A_n}{A_{n-1}}$, the $\widetilde{\Upsilon}$ matrix is symmetric,

$$x\widetilde{\tau}\left(x\right) = \widetilde{\Upsilon}\widetilde{\tau}\left(x\right) + \frac{1}{A_n}\widetilde{\pi}_n\left(x\right)e_n$$

where the vector $\widetilde{\tau}\left(x\right) = \text{diag}\left(\|\pi_j\|^{-1}\right)\tau\left(x\right)$.

If there exist two different similarity transforms H_1 and H_2 that transform a matrix A into a two different symmetric matrices, B_1 and B_2, such that $B_1 = H_1 A H_1^{-1}$ and $B_2 = H_2 A H_2^{-1}$, then $H_1^T H_1 = H_2^T H_2$. Indeed,

$$A = H_1^{-1}B_1 H_1 = H_2^{-1}B_2 H_2$$

from which $B_1 = H_1 H_2^{-1} B_2 H_2 H_1^{-1}$. Since $B_1 = B_1^T$ and $B_2 = B_2^T$, we have that

$$B_1 = \left(H_2 H_1^{-1}\right)^T B_2 \left(H_1 H_2^{-1}\right)^T$$

Hence, $H_1 H_2^{-1} = \left(H_2 H_1^{-1}\right)^T$ and $H_2 H_1^{-1} = \left(H_1 H_2^{-1}\right)^T$, which lead to $H_1^T H_1 = H_2^T H_2$. If H_1 and H_2 are, in addition, also symmetric as in the case of a diagonal matrix, then $H_1^2 = H_2^2$ or $H_1 = \pm H_2$. Since $\widetilde{\pi}_j\left(x\right) = \pi_j\left(x\right)\|\pi_j\|^{-1}$, both similarity transforms H_1 and H_2 must be the same. This implies that $H = \text{diag}\left(\sqrt{b_j}\right) = \text{diag}\left(\|\pi_j\|^{-1}\right)$, thus $b_j = \|\pi_j\|^{-2} = \frac{1}{\left(\pi_j,\pi_j\right)}$. In addition, in agreement with **art. 247**, we have

$$b_{j-1;j} = -\frac{B_j}{A_j}$$

$$\sqrt{b_{j-1;j+1}b_{j;j}} = \frac{1}{A_j}$$

Hence, transforming Υ by a similarity transform H to a symmetric matrix $\widetilde{\Upsilon}$ corresponds to normalizing the orthogonal polynomials.

262. Gerschgorin's Theorem 36 tells us that there lies a zero z_k of $\pi_n\left(x\right)$ in a disk centered around $b_{j-1;j} = -\frac{B_j}{A_j}$ with radius $\frac{1}{A_{j-1}} + \frac{1}{A_j}$. Overall, the symmetric matrix $\widetilde{\Upsilon}$ leads to the sharpest bounds on the eigenvalues/zeros of $\pi_n\left(x\right)$ because the above similarity transform H minimizes the off diagonal elements. However, not always. In particular, ignoring the attempt to symmetrize Υ, we may choose h_1 and h_n in such a way that $\left(H\Upsilon H^{-1}\right)_{12}$ and $\left(H\Upsilon H^{-1}\right)_{n;n-1}$ are arbitrarily small (but not zero). But, by making h_1 and h_n very small, we increase the radius around $b_{0;1}$ and $b_{n-1;n}$. Gerschgorin's Theorem 36 indicates that there is a zero z_k close to $b_{0;1}$ and another zero close to $b_{n-1;n}$.

263. *Continued fraction associated to orthogonal polynomials.* By systematic row multiplication and subtraction from the next one, we can eliminate the lower diagonal elements $\widetilde{\Upsilon}_{j-1;j}$ in the determinant $\det\left(\widetilde{\Upsilon} - xI\right)$, which eventually results in

a continued fraction expansion of $T_n = \det\left(\widetilde{\Upsilon} - xI\right) = \left|\widetilde{\Upsilon} - xI\right|$,

$$
T_n = \begin{vmatrix}
-\frac{B_1}{A_1} - x & \frac{1}{A_1} & & & \\
\frac{1}{A_1} & -\frac{B_2}{A_2} - x & \frac{1}{A_2} & & \\
& \ddots & \ddots & \ddots & \\
& & \frac{1}{A_{n-2}} & -\frac{B_{n-1}}{A_{n-1}} - x & \frac{1}{A_{n-1}} \\
& & & \frac{1}{A_{n-1}} & -\frac{B_n}{A_n} - x
\end{vmatrix}
$$

We write the determinant T_n in block form,

$$
T_n = \begin{vmatrix}
-\frac{A_1 x + B_1}{A_1} & \frac{1}{A_1} e_1^T \\
\frac{1}{A_1} e_1 & T_{1;n}
\end{vmatrix}
$$

where the basis vector is $e_1 = (1, 0, \ldots)$ and where the matrix $T_{1;n}$ is obtained by deleting the first row and the first column in $\widetilde{\Upsilon} - xI$,

$$
T_{1;n} = \begin{bmatrix}
-\frac{A_2 x + B_2}{A_2} & \frac{1}{A_2} & & & \\
\frac{1}{A_2} & -\frac{A_3 x + B_3}{A_3} & \frac{1}{A_3} & & \\
& \ddots & \ddots & \ddots & \\
& & \frac{1}{A_{n-2}} & -\frac{A_{n-1} x + B_{n-1}}{A_{n-1}} & \frac{1}{A_{n-1}} \\
& & & \frac{1}{A_{n-1}} & -\frac{A_n x + B_n}{A_n}
\end{bmatrix}
$$

Invoking (8.79) yields

$$
T_n = -\frac{A_1 x + B_1}{A_1} \left| T_{1;n} + \frac{1}{A_1} \frac{e_1 e_1^T}{A_1 x + B_1} \right|
$$

and $e_1 e_1^T = \widehat{O}$ equals the zero matrix (with same dimensions as T_{n-1}), except for the element $\widehat{O}_{11} = 1$. Thus,

$$
T_n = -\frac{A_1 x + B_1}{A_1} \begin{vmatrix}
-\frac{A_2 x + B_2}{A_2} + \frac{1}{A_1} \frac{1}{A_1 x + B_1} & \frac{1}{A_2} e_1^T \\
\frac{1}{A_2} e_1 & T_{2;n}
\end{vmatrix}
$$

where we denote by $T_{j;n}$ the matrix obtained by deleting the first j rows and the first j columns in $\widetilde{\Upsilon} - xI$. Again invoking (8.79) yields, with $C_n = \frac{A_n}{A_{n-1}}$,

$$
T_n = \frac{A_1 x + B_1}{A_1 A_2} \left(A_2 x + B_2 - \frac{C_2}{A_1 x + B_1} \right) \begin{vmatrix}
-\frac{A_3 x + B_3}{A_3} + \frac{1}{A_2} \frac{1}{A_2 x + B_2 - \frac{C_2}{A_1 x + B_1}} & \frac{1}{A_3} e_1^T \\
\frac{1}{A_3} e_1 & T_{3;n}
\end{vmatrix}
$$

Next,

$$
T_n = -\frac{A_1 x + B_1}{A_1 A_2 A_3} \left((A_2 x + B_2) - \frac{C_2}{A_1 x + B_1} \right) \left((A_3 x + B_3) - \frac{C_3}{A_2 x + B_2 - \frac{C_2}{A_1 x + B_1}} \right)
$$

$$
\times \begin{vmatrix}
-\frac{A_4 x + B_4}{A_4} + \frac{1}{A_3} \frac{1}{A_3 x + B_3 - \frac{C_3}{A_2 x + B_2 - \frac{C_2}{A_1 x + B_1}}} & \frac{1}{A_4} e_1^T \\
\frac{1}{A_4} e_1 & T_{4;n}
\end{vmatrix}
$$

from which we deduce that

$$T_n = \frac{(-1)^n}{\prod\limits_{k=1}^{n} A_k} \prod_{k=1}^{n} \theta_k(x)$$

where the continued fraction $\theta_k(x)$ equals

$$\theta_k(x) = A_k x + B_k - \cfrac{C_k}{A_{k\ 1}x + B_{k\ 1} - \cfrac{C_{k\ 1}}{A_{k\ 2}x + B_{k\ 2} - \cfrac{C_{k\ 2}}{\ddots\ \cfrac{\ddots}{A_2 x + B_2}\ \cfrac{C_2}{A_1 x + B_1}}}} \qquad (10.29)$$

The continued fraction thus satisfies the recursion[4]

$$\theta_k(x) = A_k x + B_k - \frac{C_k}{\theta_{k\ 1}(x)} \qquad (10.30)$$

Art. 260 shows that the characteristic polynomial $T_n = \det\left(\widetilde{\Upsilon} - xI\right)$ has the same zeros of $\pi_n(x)$, such that $T_n = \frac{(\ 1)^n}{c_{n;n}} \pi_n(x)$, and

$$\pi_n(x) = \frac{c_{n;n}}{\prod\limits_{k=1}^{n} A_k} \prod_{k=1}^{n} \theta_k(x)$$

from which,

$$\theta_n(x) = \frac{A_n c_{n\ 1;n\ 1}}{c_{n;n}} \frac{\pi_n(x)}{\pi_{n\ 1}(x)} = \frac{\widetilde{\pi}_n(x)}{\widetilde{\pi}_{n\ 1}(x)}$$

Introducing $\theta_n(x) = \frac{\widetilde{\pi}_n(x)}{\widetilde{\pi}_{n\ 1}(x)}$ into the recursion (10.30) again leads to the normalized three term recursion (10.13).

More results on continued fractions are presented in Gautschi (2004) and in Chihara (1978).

264. If $\widetilde{\Upsilon}$ is positive semidefinite, then $\widetilde{\Upsilon}$ can be considered as a Gram matrix (**art.** 175), i.e. $\widetilde{\Upsilon} = A^T A$ where $\widetilde{\Upsilon}_{i,i} \geq 0$. **Art.** 260 demonstrates that $\widetilde{\Upsilon}$ is positive semidefinite if all zeros of the orthogonal polynomials are non negative. Theorem

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[4] In most textbooks, a finite continued fraction is written in a differently labeled form as

$$\theta_n \quad a_0 \quad \cfrac{b_1}{a_1 \quad \cfrac{b_2}{a_2 - \cfrac{b_3}{\ddots\ \cfrac{b_n}{a_n}}}}$$

from which the recursive structure is less naturally observed. If the determinant T_n is expanded by the last row and last column, up to the first one, a same labeling would have been found. The main purpose in classical treatment to use the highest index in the deepest fraction is to study the convergence of $\lim_{n\to\infty} \theta_n$.

66 guarantees semidefiniteness when the orthogonality interval $[a, b]$ lies on the non negative real axis, i.e., if $b > a \geq 0$.

Since $\widetilde{\Upsilon}$ is a three band matrix, A is a two band matrix with diagonal elements $A_{jj} = a_j$ for $1 \leq j \leq n$ and upper diagonal elements $A_{j,j+1} = b_j$ for $1 \leq j \leq n-1$. Indeed,

$$\widetilde{\Upsilon}_{ij} = \sum_{k=1}^{n} \left(A^T\right)_{ik} A_{kj} = \sum_{k=1}^{n} A_{ki} A_{kj}$$

$$= A_{ii} A_{ij} + A_{i\ 1,i} A_{i\ 1,j} = a_i A_{ij} + b_{i\ 1} A_{i\ 1,j}$$

and

$$\widetilde{\Upsilon}_{ij} = \begin{cases} a_{i\ 1} b_{i\ 1} & \text{if } j = i - 1 \\ a_i^2 + b_{i\ 1}^2 & \text{if } j = i \\ a_i b_i & \text{if } j = i + 1 \end{cases}$$

Hence, if $i = 1$, comparison shows that $\widetilde{\Upsilon}_{11} = a_1^2$ and $\widetilde{\Upsilon}_{12} = a_1 b_1$ such that $a_1 = \sqrt{-\frac{B_1}{A_1}}$ and $b_1 = \frac{1}{\sqrt{B_1 A_1}}$. For the i th row, we find the equations

$$\widetilde{\Upsilon}_{i,i\ 1} = a_{i\ 1} b_{i\ 1} = \frac{1}{A_{i\ 1}}$$

$$\widetilde{\Upsilon}_{i,i} = a_i^2 + b_{i\ 1}^2 = -\frac{B_i}{A_i}$$

$$\widetilde{\Upsilon}_{i,i+1} = a_i b_i = \frac{1}{A_i}$$

whose solution, by iteration from $i = 1$, is a continued fraction

$$a_j^2 = -\frac{B_j}{A_j} + \cfrac{1}{A_{j\ 1} B_{j\ 1} - \cfrac{A_{j\ 1}^2}{A_{j\ 2} B_{j\ 2} - \cfrac{A_{j\ 2}^2}{A_{j\ 3} B_{j\ 3} - \cfrac{A_{j\ 3}^2}{\ddots \quad \cfrac{\ddots}{A_2 B_2 \quad \frac{A_2^2}{A_1 B_1}}}}}}$$

$$b_j^2 = \cfrac{1}{-A_j B_j + \cfrac{A_j^2}{A_{j\ 1} B_{j\ 1} - \cfrac{A_{j\ 1}^2}{A_{j\ 2} B_{j\ 2} - \cfrac{A_{j\ 2}^2}{A_{j\ 3} B_{j\ 3} - \cfrac{A_{j\ 3}^2}{\ddots \quad \cfrac{\ddots}{A_2 B_2 \quad \frac{A_2^2}{A_1 B_1}}}}}}}$$

satisfying the recursion $a_j^2 = -\frac{B_j}{A_j} - \frac{1}{A_{j\ 1}^2 a_{j\ 1}^2}$. Either the positive square root $\left(\sqrt{a_j^2}, \sqrt{b_j^2}\right)$ in both or the negative square root $\left(-\sqrt{a_j^2}, -\sqrt{b_j^2}\right)$ are solutions. By comparison with the continued fraction (10.29) where $C_n = \frac{A_n}{A_{n\ 1}}$, we verify that

$$a_j^2 = -\frac{\theta_j(0)}{A_j} \quad \text{and} \quad b_j^2 = -\frac{1}{A_j \theta_j(0)}$$

In summary, the matrix A, which satisfies $\widetilde{\Upsilon} = A^T A$, is

$$A = \begin{bmatrix} a_1 & b_1 & & & \\ 0 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & a_{n-1} & b_{n-1} \\ & & & 0 & a_n \end{bmatrix}$$

The eigenvalues of A are its diagonal elements a_i. The eigenvector x_i of A belonging to $\lambda = a_i$ can be written explicitly: just write out $Ax_i = a_i x_i$, starting with the last component $(x_i)_n = 1_{\{i=n\}}$, and iterate upwards. Thus, $A = X \mathrm{diag}(\lambda(A)) X^{-1}$ can be explicitly written where X is the matrix with as columns its eigenvectors, and

$$\widetilde{\Upsilon} = A^T A = \left(X^{-1} \right)^T \mathrm{diag} \left(\lambda \left(A \right) \right) X^T X \mathrm{diag} \left(\lambda \left(A \right) \right) X^{-1}$$

After eigenvalue decomposition, the symmetric matrix

$$\widetilde{\Upsilon} = U \mathrm{diag} \left(\lambda_k \left(\widetilde{\Upsilon} \right) \right) U^{-1}$$

where $U^T = U^{-1}$ (or $U^T U = U U^T = I$) is an orthogonal matrix (**art. 151**). The latter is a property of symmetric matrices and does not hold in general. Hence, X is not necessary orthogonal, although the eigenvectors $x_1, x_2, \ldots, x_n$ of A are linearly independent. Since $\widetilde{\Upsilon}$ is positive semidefinite, $\lambda_k \left(\widetilde{\Upsilon} \right) \geq 0$ and, thus $\sqrt{\lambda_k \left(\widetilde{\Upsilon} \right)}$ is real such that

$$\widetilde{\Upsilon} = U \mathrm{diag} \left(\lambda_k \left(\widetilde{\Upsilon} \right) \right) U^{-1} = U \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) Y^T Y \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) U^T$$

$$= U \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) Y^T \left(U \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) Y^T \right)^T$$

where Y is an orthogonal matrix. Hence, we can construct the matrix $A = Y \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) U^T$, which is a singular value decomposition[5]. Obviously, the simplest choice is $Y = I$, in which case, $A = \mathrm{diag} \left(\sqrt{\lambda_k(\widetilde{\Upsilon})} \right) U^T$. However, mul

tiplication by a diagonal matrix only multiplies row j in U^T by $\sqrt{\lambda_j(\widetilde{\Upsilon})}$ and the resulting structure should be the two band structure of A. Since the two band structure of A is not orthogonal (the column vectors in A are not orthogonal), $Y = I$ is not a correct choice. Also, $Y \neq U$, because A is not symmetric. Applying QR decomposition (see, e.g., Golub and Van Loan (1996)) to $A = X \mathrm{diag}(\lambda(A)) X^{-1}$ with $X = QR$ and $X^{-1} = R_1 Q_1^T$ yields

$$A = QR \mathrm{diag} \left(\lambda \left(A \right) \right) R_1 Q_1^T$$

---

[5] Although the singular values are unique, the singular vectors are not, and, hence $A = U\Sigma V^T$ is not unique.

Since $A = Y\text{diag}\left(\sqrt{\lambda_k(\widetilde{\Upsilon})}\right) U^T$, it remains to show that $R\text{diag}(\lambda(A)) R_1$ is a diagonal matrix. Unfortunately, the major difficulty is to find an orthogonalization process for the eigenvectors X such that $A = X\text{diag}(\lambda(A)) X^{-1}$ has a singular value decomposition $A = Y\text{diag}\left(\sqrt{\lambda_k(\widetilde{\Upsilon})}\right) U^T$. There does not exist a general method to achieve this result. If it existed, we would have, at least for the class of orthogonal polynomials with zeros on the positive real axis, a general method to compute the exact zeros!

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