GRAPH SPECTRA FOR COMPLEX NETWORKS

This concise and self-contained introduction builds up the spectral theory of graphs from scratch, with linear algebra and the theory of polynomials developed in the later parts. The book focuses on properties and bounds for the eigenvalues of the adjacency, Laplacian and effective resistance matrices of a graph. The goal of the book is to collect spectral properties that may help to understand the behavior or main characteristics of real-world networks. The chapter on spectra of complex networks illustrates how the theory may be applied to deduce insights into real-world networks.

The second edition contains new chapters on topics in linear algebra and on the effective resistance matrix, and treats the pseudoinverse of the Laplacian. The latter two matrices and the Laplacian describe linear processes, such as the flow of current, on a graph. The concepts of spectral sparsification and graph neural networks are included.

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Cambridge University Press & Assessment
978-1-009-36680-9 — Graph Spectra for Complex Networks
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Second Edition

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CAMBRIDGE
UNIVERSITY PRESS

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Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre,
New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment,
a department of the University of Cambridge.

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www.cambridge.org
Information on this title: www.cambridge.org/9781009366809

DOI: 10.1017/9781009366793

First published 2011
Second edition 2023

A catalogue record for this publication is available from the British Library

A Cataloging-in-Publication data record for this book is available from the Library of Congress

ISBN 978-1-009-36680-9 Paperback

in memory of Saskia and Nathan

to Huijuan

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Preface to the second edition

There is no place for ugly mathematics (G. H. Hardy)

After more than a decade, a new edition was felt needed. The interest in and the role of networks is still increasing, although the landscape of graph spectra is not dramatically changed, but is slowly evolving. New theory or theory that I have missed in the first edition is added. For example, I include the matrix theory of linear processes on a graph, whose dynamics is proportional to the underlying topology, such as fluids flowing in a network of pipes or electrical current in a resistor network. The vector of the injected current at nodes is connected to the vector of potentials at those nodes by a weighted Laplacian as explained in **art**. 14, from which the pseudoinverse of the Laplacian naturally arises. The physics and meaning of the diagonal elements of the pseudoinverse as well as the effective resistance matrix of a graph are treated in Chapter 5.

The computation of graph spectra, eigenvalues and eigenvectors requires the theory of linear algebra and polynomials. In the first edition, the book was divided into two parts, where the second part originated from exploded appendices. This second edition consists of three parts. The core of the book is Part I on Spectra of Graphs, which consumes more than half of the pages and seven chapters. The main theory on the eigenvalue equation (1.3), that comprises matrix and determinant operations in linear algebra, is summarized in the Eigensystem in Part II. The theory of polynomials, which also belongs to function theory, is contained in Part III. Those two last parts contain the general theory, which is applied to graphs in Part I. The reason for the separation is the inclusion of many nice results that make those two last parts self-contained. Parts II and III can be read independently of Part I.

Apart from the correction of errors and the deletion of a few articles (**art.**) in the first edition, many additions have been included in this second edition. Some additions are new and not published before. The list of new material in this second edition is:

in Chapter 2: **art**. 12, 13, 14 to 16, 28, 29, 33, 35, 38 to 40, 17, 19, 21 to 24;
in Chapter 3: **art**. 43, 44, 52 to 58, 61, 64, 70, 71, 81, 87 to 91, 93 98;
in Chapter 4: **art**. 118, 120, 128 to 132, 139, 160, 161;
Chapter 5 on the effective resistance matrix;
in Chapter 6: Sections 6.4.3, 6.11 and 6.12;
in Chapter 7: **art**. 172, 182 and Section 7.5.3;
in Chapter 8: Sections 8.8 to 8.11;
Chapter 9 contains matrix transformations and properties of the determinant;

in Chapter 10: **art**. 240, 241, 248, 249, 253, 256, 257, 258, 259, 271, 281 and Sections 10.2, 10.7 and 10.10;

in Chapter 11: **art**. 293, 304, 305, 308, 312, 334, 336 and Section 11.6;

and in Chapter 12: Section 12.7.

Just as in the first edition, the main focus is on undirected graphs, whose graph-related matrices as the adjacency matrix and Laplacian are symmetric. For symmetric matrices, the eigenvalue decomposition is effective, simple and beautiful. Asymmetic matrices such as the non-backtracking matrix and the Markovian transition probability matrix specifying the directed Markov graph are not treated. Another omission concerns eigenvectors of graph-related matrices. Apart from their computation, relatively little is understood about eigenvectors, although we expect that progress will occur in the near future. A reason for this belief is the discovery of the geometric simplex representation of an undirected graph, which is a third equivalent representation besides the topology and the spectral domain, explained in the Preface to the first edition below. Any undirected graph, possibly weighted, on N nodes is a simplex – a generalization of a triangle in higher dimensions than two – in the $N-1$ dimensional Euclidean space, as first deduced by Fiedler (2009) and rediscovered by us (Devriendt and Van Mieghem, 2019a) while studying electrical resistor networks. That simplex is intimately related to eigenvectors of the Laplacian matrix, but we omit the simplex geometry of a graph and simplicial complexes. A last omission is specific topics in the relatively new field of graph signal processing, for which we refer to the recent book by Ortega (2022) and Section 8.11 for the concepts of graph neural networks. Graph signal processing analyzes data generated by processes on graphs and its aim is similar to that of Network Science; roughly the same topics are treated, only the approach and nomenclature differs somewhat. Here, we follow the network science terminology. While this book contains inequalities for eigenvalues of graph-related matrices, Stanić (2015) devotes an entire book on eigenvalue inequalities, which complements ours.

Finally, I hope that this new edition is easier to read: cross-referencing between articles **art.** is greatly improved and I have tried to fabricate many **art.**'s as more independent blocks that can stand on their own. To increase the readability, the equation labels in Part II and III contain as first indicator A and B, respectively, instead of the chapter number that is maintained in the core Part I.

July 2023 PIET VAN MIEGHEM

Cambridge University Press & Assessment
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Preface to the first edition

During the first years of the third millennium, considerable interest arose in complex 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 augmenting 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 networks. 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 represented 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 meaning 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 segment 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 inherent 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.** 247.

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 examples 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 produced over time. Some properties of the signal are more appropriately studied in the time-domain, while others are in the transformed domain, the frequency domain. 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 (2008) 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 91 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.

I would like to thank Huijuan Wang, for her general interest, input and help in pointing me to interesting articles. Further, I am most grateful to Fernando Kuipers for proofreading the first version of the manuscript, to Roeloef Koekoek for reviewing Chapter 12 on orthogonal polynomials, and to Jasmina Omic for the numerical evaluation of bounds on the largest eigenvalue of the adjacency matrix. Javier Martin Hernandez, Dajie Liu and Xin Ge have provided me with many nice pictures of graphs and plots of spectra. Stojan Trajanovski has helped me with the m-dimensional lattice and **art.** 153. Wynand Winterbach showed that the assortativity of regular graphs is not necessarily equal to one, by pointing to the example of the complete graph minus one link (Section 8.5.1.1). Rob Kooij has constructed Fig. 4.1 as a counter example for the common belief that Fiedler's algebraic connectivity is always an adequate metric for network robustness with respect to graph disconnectivity. As in my previous book (Van Mieghem, 2006), David Hemsley has suggested a number of valuable textual improvements.

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

I would like to thank Massimo Achterberg and Xiangrong Wang for numerous comments and corrections. Hale Cetinay has contributed to the pseudoinverse of the Laplacian (Section 4.2). Karel Devriendt has informed me about several results in the literature that were unknown to me and he has derived new results in Section 5.2 on the effective resistance. Moreover, Karel also continued to show me his own new inventions, about eigenvectors of the Laplacian and about effective resistances, after he left our group NAS at Delft University of Technology. Further, Albert Cenen Cerda, Bastian Prasse, Qiang Liu and Jaron Sanders have read chapters together during several weeks around the end of 2018 and beginning of 2019 and provided me with a list of errors and suggested improvements. Ivan Jokić has derived the Hadamard product identity in **art.** 96.

I am very pleased that Massimo Achterberg, Scott Dalhgren, Clare Dennison, Karel Devriendt, Johan Dubbeldam, Ivan Jokić, Yingyue Ke, Rob Kooij, Geert Leus, Rogier Noldus, Bastian Prasse and Dragan Stevanović have read several chapters, pointed me to errors and provided input on the final version, just before publication.

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 a complex number. Also the element a_{ij} of a matrix A is written with a small letter. 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 {.}. The largest integer smaller than or equal to x is denoted by $\lfloor x \rfloor$, whereas $\lceil x \rceil$ equals the smallest integer larger than or equal to x.

Linear Algebra

A	$n \times m$ matrix $\begin{bmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & & \\ a_{n1} & \ldots & a_{nm} \end{bmatrix}$
$\det A$	$= \begin{vmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \\ a_{n1} & \ldots & a_{nn} \end{vmatrix}$: determinant of a square matrix A
$\text{trace}(A)$	$= \sum_{j=1}^{n} a_{jj}$: sum of diagonal elements of A
$\text{diag}(a)$	$= \text{diag}(a_1, a_2, \ldots, a_n)$: diagonal matrix with diagonal elements equal to the components of the vector $a = (a_1, a_2, \ldots, a_n)$ while all off-diagonal elements are zero
A^T	transpose of a matrix, the rows of A are the columns of A^T
A^*	matrix in which each element is the complex conjugate of the corresponding element in A
A^H	$= (A^*)^T$: Hermitian of matrix A
$c_A(x)$	$= \det(A - xI)$: characteristic polynomial of A
$\text{adj}A$	$= A^{-1} \det A$: adjugate of A

AB	matrix product of $n \times m$ matrix A and $m \times l$ matrix B with element $(AB)_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$
$A \circ B$	Hadamard product of $n \times n$ matrix A and $n \times n$ matrix B with element $(A \circ B)_{ij} = a_{ij} b_{ij}$
J	all-one matrix
u	all-one vector
I	diag(u), identity matrix
$Q(\lambda)$	$= \frac{c_A(\lambda)}{\lambda I - A}$: adjoint of A
e_j	basic vector: all components are zero, except component j is 1
δ_{kj}	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 graph G
$\mathcal{N}$	set of nodes in graph G
L	$= \lvert\mathcal{L}\rvert$: number of links in graph G
N	$= \lvert\mathcal{N}\rvert$: number of nodes in graph G
A	adjacency matrix of graph G
B	incidence matrix of graph G
Q	$= BB^T$ Laplacian matrix of graph G
$Q^\dagger$	pseudoinverse of the Laplacian matrix of graph G
Ω	effective resistance matrix of graph G
H	hopcount in a graph (random variable) or hopcount matrix
$l(G)$	line graph of graph G
Δ	$= \text{diag}(d)$: diagonal matrix of the nodal degrees
d	degree vector of a graph G
d_j	degree of node j
$d_{(j)}$	the j-th largest degree of node in graph G

$d_{\max}$	maximum degree in graph G
$d_{\min}$	minimum degree in graph G
D	degree (random variable) in graph G
$\kappa_{\mathcal{N}}(G)$	vertex (node) connectivity of graph G
$\kappa_{\mathcal{L}}(G)$	edge (link) connectivity of graph G
R_G	effective graph resistance
$\blacktriangle_G$	the number of triangles in graph G
$\{\lambda_k\}_{1\leq k\leq N}$	set of eigenvalues of A ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$
$\{\mu_k\}_{1\leq k\leq N}$	set of eigenvalues of Q ordered as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_N$
N_k	total number of walks with length k
W_k	number of closed walks with length k
ρ	diameter of graph G
ρ_D	degree assortativity of graph G
ω	clique number of graph G
K_N	the complete graph with N nodes
$K_{n,m}$	the complete bi-partite graph with $N = n + m$
P_N	path on N nodes