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Carlos Hoppen · David P. Jacobs · Vilmar Trevisan

Locating Eigenvalues in Graphs

Algorithms and Applications

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Carlos Hoppen
Instituto de Matemática e Estatística
Universidade Federal do Rio Grande do Sul
Porto Alegre, Rio Grande do Sul, Brazil

David P. Jacobs
School of Computing
Clemson University
Clemson, SC, USA

Vilmar Trevisan
Instituto de Matemática e Estatística
Universidade Federal do Rio Grande do Sul
Porto Alegre, Rio Grande do Sul, Brazil

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À Prof[a]. Nair Abreu, cujo entusiasmo e generosidade nos trouxe à Teoria Espectral dos Grafos.

Ao Prof. Underwood Dudley, por nos revelar a beleza das demonstrações.

V. Trevisan também dedica este livro à Eliana, sua companheira de vida.

Preface

Spectral graph theory is a research area that combines tools and concepts of linear algebra and combinatorics. Its main goal is to determine properties of a graph through the eigenvalues and eigenvectors of matrices associated with it.

Perhaps surprisingly, eigenvalues and eigenvectors turn out to be intimately connected with the structure of a graph. In terms of applications, they have proved to be useful for isomorphism testing and embedding graphs in the plane, for graph partitioning and clustering, as topological descriptors for networks and molecules, in the geometric description of data sets, and in the design of efficient networks, just to mention a few. In a purely mathematical perspective, the study of graph spectra has led to a myriad of open problems, ranging from the construction of graphs with a given set of eigenvalues to extremal problems that ask for a characterization of graphs that maximize or minimize some spectral parameter.

Of course, computing these eigenvalues and eigenvectors is a necessary step in any such application. Since eigenvalues are the roots of a polynomial, in general we cannot expect to find simple expressions for these roots. However, there are numerical algorithms that allow us to approximate them with any desired precision in polynomial time.

In 2011 a linear time algorithm was discovered for deciding how many eigenvalues of the adjacency matrix of a tree lie in any interval. In addition to being fast and easy to implement, this algorithm is surprisingly simple and, at first glance, does not seem to be acting on matrices. Its underlying idea was soon extended to deal with other matrices and graph classes, giving rise to the systematic study of what we now call *eigenvalue location algorithms*.

More than being a practical way of approximating eigenvalues, these algorithms have shown to be instrumental to settle theoretical questions involving the distribution of eigenvalues in graphs in a given class. In particular, an eigenvalue location algorithm was the main tool for the recent solution of a difficult conjecture involving the distribution of Laplacian eigenvalues in trees.

In this book, we survey the evolution of eigenvalue location algorithms in an organized and unified way, starting with algorithms for trees and other well-known graph classes, such as cographs, and showing how they motivated more recent algorithms that may be applied to arbitrary graphs, but whose efficiency depends on the existence of a graph decomposition of low complexity. While they are vastly deeper than the simple tree algorithm, we wish to convince the readers that they are similar in spirit.

This book is intended for graduate students and researchers in spectral graph theory. We have strived to make it as self-contained as possible. This has led to a book that combines a compact introduction to spectral graph theory with a discussion of structural decompositions such as tree decompositions and clique decompositions, which is rarely explored by books in this area. We hope that it may be used as a concise introduction to eigenvalue location algorithms for researchers who wish to know more about eigenvalues associated with graphs.

Porto Alegre, Brazil — Carlos Hoppen
Clemson, SC, USA — David P. Jacobs
Porto Alegre, Brazil — Vilmar Trevisan
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We are also thankful to three anonymous reviewers, whose careful reading and thoughtful considerations have led to a better book.

Many of the figures in this book were made using TikZiT, a program for drawing graphs, making the construction of such figures simple and straightforward.

Contents

Chapter 1
Introduction

Eigenvalues are numbers that are associated with matrices and have been of interest to mathematicians for over two hundred years. They seem to come up in almost every branch of science, including biology [1], chemistry [21], epidemiology [14, 22], geology [20], data science [13], dynamical systems [7], and network design [3]. As of this writing, a search for the word *eigenvalue* in the MathSciNet database of the American Mathematical Society returns 87,293 matches.

Spectral graph theory seeks to study graphs through the eigenvalues and eigenvectors of matrices associated with them. For example, just looking at the multiset of eigenvalues, or *spectrum*, of the adjacency and Laplacian matrices associated with a graph, we are able to tell its number of vertices, edges, and triangles, how many components it has, whether it is bipartite or not, among many other things. Even parameters that are hard to compute, such as the domination number, the chromatic number or the independence number of a graph G, can often be bounded in terms of certain eigenvalues of matrices associated with G.

The eigenvalues of a matrix are precisely the roots of the so-called *characteristic polynomial*, which, for an $n \times n$ matrix, has degree n and can generally be constructed efficiently. The problem of finding the roots of a polynomial, also known as solving an algebraic equation, is very old and has played a fundamental role in the evolution of mathematics since ancient history. The quest for algorithms that find the solutions to these equations continued through the middle ages and the first centuries of modern history and culminated with the work of 19th century mathematicians such as Abel and Galois, who proved groundbreaking results showing that there is no general formula for the roots of polynomials with integer coefficients having degree five or more. Nowadays, there are powerful numerical algorithms that are able to approximate the eigenvalues with any given precision in cubic time [16].

In this book, we address the problem of computing eigenvalues in terms of *eigenvalue location*, by which we mean determining the number of eigenvalues of

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