

GERAD

Groupe d'études et de recherche en analyse des décisions

GRAPH THEORY AND COMBINATORIAL OPTIMIZATION

Edited by
David Avis
Alain Hertz
Odile Marcotte



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Edited by

DAVID AVIS

McGill University and GERAD

ALAIN HERTZ

École Polytechnique de Montréal and GERAD

ODILE MARCOTTE

Université du Québec à Montréal and GERAD



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David Avis
McGill University & GERAD
Montréal, Canada

Alain Hertz
École Polytechnique de Montréal & GERAD
Montréal, Canada

Odile Marcotte
Université du Québec à Montréal and GERAD
Montréal, Canada

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GRAPH THEORY AND COMBINATORIAL OPTIMIZATION

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David Avis, Alain Hertz, and Odile Marcotte, editors
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Foreword

GERAD celebrates this year its 25th anniversary. The Center was created in 1980 by a small group of professors and researchers of HEC Montréal, McGill University and of the École Polytechnique de Montréal. GERAD's activities achieved sufficient scope to justify its conversion in June 1988 into a Joint Research Centre of HEC Montréal, the École Polytechnique de Montréal and McGill University. In 1996, the Université du Québec à Montréal joined these three institutions. GERAD has fifty members (professors), more than twenty research associates and post doctoral students and more than two hundreds master and Ph.D. students.

GERAD is a multi-university center and a vital forum for the development of operations research. Its mission is defined around the following four complementarily objectives:

- The original and expert contribution to all research fields in GERAD's area of expertise;
- The dissemination of research results in the best scientific outlets as well as in the society in general;
- The training of graduate students and post doctoral researchers;
- The contribution to the economic community by solving important problems and providing transferable tools.

GERAD's research thrusts and fields of expertise are as follows:

- Development of mathematical analysis tools and techniques to solve the complex problems that arise in management sciences and engineering;
- Development of algorithms to resolve such problems efficiently;
- Application of these techniques and tools to problems posed in related disciplines, such as statistics, financial engineering, game theory and artificial intelligence;
- Application of advanced tools to optimization and planning of large technical and economic systems, such as energy systems, transportation/communication networks, and production systems;
- Integration of scientific findings into software, expert systems and decision-support systems that can be used by industry.

One of the marking events of the celebrations of the 25th anniversary of GERAD is the publication of ten volumes covering most of the Center's research areas of expertise. The list follows: **Essays and Surveys in Global Optimization**, edited by C. Audet, P. Hansen and G. Savard; **Graph Theory and Combinatorial Optimization**,

edited by D. Avis, A. Hertz and O. Marcotte; **Numerical Methods in Finance**, edited by H. Ben-Ameur and M. Breton; **Analysis, Control and Optimization of Complex Dynamic Systems**, edited by E.K. Boukas and R. Malhamé; **Column Generation**, edited by G. Desaulniers, J. Desrosiers and M.M. Solomon; **Statistical Modeling and Analysis for Complex Data Problems**, edited by P. Duchesne and B. Rémillard; **Performance Evaluation and Planning Methods for the Next Generation Internet**, edited by A. Girard, B. Sansò and F. Vázquez-Abad; **Dynamic Games: Theory and Applications**, edited by A. Haurie and G. Zaccour; **Logistics Systems: Design and Optimization**, edited by A. Langevin and D. Riopel; **Energy and Environment**, edited by R. Loulou, J.-P. Waaub and G. Zaccour.

I would like to express my gratitude to the Editors of the ten volumes, to the authors who accepted with great enthusiasm to submit their work and to the reviewers for their benevolent work and timely response. I would also like to thank Mrs. Nicole Paradis, Francine Benoît and Louise Letendre and Mr. André Montpetit for their excellent editing work.

The GERAD group has earned its reputation as a worldwide leader in its field. This is certainly due to the enthusiasm and motivation of GERAD's researchers and students, but also to the funding and the infrastructures available. I would like to seize the opportunity to thank the organizations that, from the beginning, believed in the potential and the value of GERAD and have supported it over the years. These are HEC Montréal, École Polytechnique de Montréal, McGill University, Université du Québec à Montréal and, of course, the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Fonds québécois de la recherche sur la nature et les technologies (FQRNT).

Georges Zaccour
Director of GERAD

Avant-propos

Le Groupe d'études et de recherche en analyse des décisions (GERAD) fête cette année son vingt-cinquième anniversaire. Fondé en 1980 par une poignée de professeurs et chercheurs de HEC Montréal engagés dans des recherches en équipe avec des collègues de l'Université McGill et de l'École Polytechnique de Montréal, le Centre comporte maintenant une cinquantaine de membres, plus d'une vingtaine de professionnels de recherche et stagiaires post-doctoraux et plus de 200 étudiants des cycles supérieurs. Les activités du GERAD ont pris suffisamment d'ampleur pour justifier en juin 1988 sa transformation en un Centre de recherche conjoint de HEC Montréal, de l'École Polytechnique de Montréal et de l'Université McGill. En 1996, l'Université du Québec à Montréal s'est jointe à ces institutions pour parrainer le GERAD.

Le GERAD est un regroupement de chercheurs autour de la discipline de la recherche opérationnelle. Sa mission s'articule autour des objectifs complémentaires suivants :

- la contribution originale et experte dans tous les axes de recherche de ses champs de compétence ;
- la diffusion des résultats dans les plus grandes revues du domaine ainsi qu'auprès des différents publics qui forment l'environnement du Centre ;
- la formation d'étudiants des cycles supérieurs et de stagiaires post-doctoraux ;
- la contribution à la communauté économique à travers la résolution de problèmes et le développement de coffres d'outils transférables.

Les principaux axes de recherche du GERAD, en allant du plus théorique au plus appliqué, sont les suivants :

- le développement d'outils et de techniques d'analyse mathématiques de la recherche opérationnelle pour la résolution de problèmes complexes qui se posent dans les sciences de la gestion et du génie ;
- la confection d'algorithmes permettant la résolution efficace de ces problèmes ;
- l'application de ces outils à des problèmes posés dans des disciplines connexes à la recherche opérationnelle telles que la statistique, l'ingénierie financière, la théorie des jeux et l'intelligence artificielle ;
- l'application de ces outils à l'optimisation et à la planification de grands systèmes technico-économiques comme les systèmes énergétiques, les réseaux de télécommunication et de transport, la logistique et la distributive dans les industries manufacturières et de service ;

- l'intégration des résultats scientifiques dans des logiciels, des systèmes experts et dans des systèmes d'aide à la décision transférables à l'industrie.

Le fait marquant des célébrations du 25^e du GERAD est la publication de dix volumes couvrant les champs d'expertise du Centre. La liste suit : **Essays and Surveys in Global Optimization**, édité par C. Audet, P. Hansen et G. Savard ; **Graph Theory and Combinatorial Optimization**, édité par D. Avis, A. Hertz et O. Marcotte ; **Numerical Methods in Finance**, édité par H. Ben-Ameur et M. Breton ; **Analysis, Control and Optimization of Complex Dynamic Systems**, édité par E.K. Boukas et R. Malhamé ; **Column Generation**, édité par G. Desaulniers, J. Desrosiers et M.M. Solomon ; **Statistical Modeling and Analysis for Complex Data Problems**, édité par P. Duchesne et B. Rémillard ; **Performance Evaluation and Planning Methods for the Next Generation Internet**, édité par A. Girard, B. Sansò et F. Vázquez-Abad ; **Dynamic Games : Theory and Applications**, édité par A. Haurie et G. Zaccour ; **Logistics Systems : Design and Optimization**, édité par A. Langevin et D. Riopel ; **Energy and Environment**, édité par R. Loulou, J.-P. Waaub et G. Zaccour.

Je voudrais remercier très sincèrement les éditeurs de ces volumes, les nombreux auteurs qui ont très volontiers répondu à l'invitation des éditeurs à soumettre leurs travaux, et les évaluateurs pour leur bénévolat et ponctualité. Je voudrais aussi remercier Mmes Nicole Paradis, Francine Benoît et Louise Letendre ainsi que M. André Montpetit pour leur travail expert d'édition.

La place de premier plan qu'occupe le GERAD sur l'échiquier mondial est certes due à la passion qui anime ses chercheurs et ses étudiants, mais aussi au financement et à l'infrastructure disponibles. Je voudrais profiter de cette occasion pour remercier les organisations qui ont cru dès le départ au potentiel et à la valeur du GERAD et nous ont soutenus durant ces années. Il s'agit de HEC Montréal, l'École Polytechnique de Montréal, l'Université McGill, l'Université du Québec à Montréal et, bien sûr, le Conseil de recherche en sciences naturelles et en génie du Canada (CRSNG) et le Fonds québécois de la recherche sur la nature et les technologies (FQRNT).

Georges Zaccour
Directeur du GERAD

Contributing Authors

NAIR MARIA MAIA DE ABREU
Universidade Federal do Rio de Janeiro,
Brasil
nair@pep.ufrj.br

SLIM BELHAIZA
École Polytechnique de Montréal,
Canada
Slim.Belhaiza@polymtl.ca

PETER BRASS
City College, City University of New
York, USA
peter@cs.cuny.cuny.edu

KOMEI FUKUDA
ETH Zurich, Switzerland
komei.fukuda@ifor.math.ethz.ch

PIERRE HANSEN
HEC Montréal and GERAD, Canada
Pierre.Hansen@gerad.ca

ALAIN HERTZ
École Polytechnique de Montréal and
GERAD, Canada
alain.hertz@gerad.ca

KARTIK KRISHNAN
McMaster University, Canada
kartik@optlab.mcmaster.ca

WIESLAW KUBIAK
Memorial University of Newfoundland,
Canada
wkubiak@mun.ca

VADIM V. LOZIN
Rutgers University, USA
lozin@rutcor.rutgers.edu

PATRICE MARCOTTE
Université de Montréal, Canada
marcotte@iro.umontreal.ca

CARLA SILVA OLIVEIRA
Escola Nacional de Ciências Estatísticas,
Brasil
carlasilva@ibge.gov.br

JÁNOS PACH
City College, City University of New
York, USA
pach@cims.nyu.edu

VERA ROSTA
Alfréd Rényi Institute of Mathematics,
Hungary & McGill University, Canada
rosta@renyi.hu

GILLES SAVARD
École Polytechnique de Montréal and
GERAD, Canada
gilles.savard@polymtl.ca

F.B. SHEPHERD
Bell Laboratories, USA
bshep@research.bell-labs.com

TAMÁS TERLAKY
McMaster University, Canada
terlaky@mcmaster.ca

A. VETTA
McGill University, Canada
vetta@math.mcgill.ca

DOMINIQUE DE WERRA
École Polytechnique Fédérale de
Lausanne, Switzerland
dewerra@dma.epfl.ch

Preface

Combinatorial optimization is at the heart of the research interests of many members of GERAD. To solve problems arising in the fields of transportation and telecommunication, the operations research analyst often has to use techniques that were first designed to solve classical problems from combinatorial optimization such as the maximum flow problem, the independent set problem and the traveling salesman problem. Most (if not all) of these problems are also closely related to graph theory. The present volume contains nine chapters covering many aspects of combinatorial optimization and graph theory, from well-known graph theoretical problems to heuristics and novel approaches to combinatorial optimization.

In Chapter 1, Belhaiza, de Abreu, Hansen and Oliveira study several conjectures on the algebraic connectivity of graphs. Given an undirected graph G , the algebraic connectivity of G (denoted $a(G)$) is the smallest eigenvalue of the Laplacian matrix of G . The authors use the AutoGraphiX (AGX) system to generate connected graphs that are not complete and minimize (resp. maximize) $a(G)$ as a function of n (the order of G) and m (its number of edges). They formulate several conjectures on the structure of these extremal graphs and prove some of them.

In Chapter 2, Brass and Pach survey the results in the theory of geometric patterns and give an overview of the many interesting problems in this theory. Given a set S of n points in d -dimensional space, and an equivalence relation between subsets of S , one is interested in the equivalence classes of subsets (i.e., *patterns*) occurring in S . For instance, two subsets can be deemed equivalent if and only if one is the translate of the other. Then a *Turán-type* question is the following: “What is the maximum number of occurrences of a given pattern in S ?” A *Ramsey-type* question is the following: “Is it possible to color space so that there is no monochromatic occurrence of a given pattern?” Brass and Pach investigate these and other questions for several equivalence relations (translation, congruence, similarity, affine transformations, etc.), present the results for each relation and discuss the outstanding problems.

In Chapter 3, Fukuda and Rosta survey various data depth measures, first introduced in nonparametric statistics as multidimensional generalizations of ranks and the median. These data depth measures have been studied independently by researchers working in statistics, political science, optimization and discrete and computational geometry. Fukuda and Rosta show that computing data depth measures often reduces to

finding a maximum feasible subsystem of linear inequalities, that is, a solution satisfying as many constraints as possible. Thus they provide a unified framework for the main data depth measures, such as the half-space depth, the regression depth and the simplicial depth. They survey the related results from nonparametric statistics, computational geometry, discrete geometry and linear optimization.

In Chapter 4, Hertz and Lozin survey the method of augmenting graphs for solving the maximum independent set problem. It is well known that the maximum matching problem can be solved by looking for augmenting paths and using them to increase the size of the current matching. In the case of the maximum independent set problem, however, finding an augmenting graph is much more difficult. Hertz and Lozin show that for special classes of graphs, all the families of augmenting graphs can be characterized and the problem solved in polynomial time. They present the main results of the theory of augmenting graphs and propose new contributions to this theory.

In Chapter 5, Krishnan and Terlaky present a survey of semidefinite and interior point methods for solving NP-hard combinatorial optimization problems to optimality and designing approximation algorithms for some of these problems. The approaches described in this chapter include non-convex potential reduction methods, interior point cutting plane methods, primal-dual interior point methods and first-order algorithms for solving semidefinite programs, branch-and-cut approaches based on semidefinite programming formulations and finally methods for solving combinatorial optimization problems by means of successive convex approximations.

In Chapter 6, Kubiak presents a study of balancing mixed-model supply chains. A *mixed-model supply chain* is designed to deliver a wide range of customized models of a product to customers. The main objective of the model is to keep the supply of each model as close to its demand as possible. Kubiak reviews algorithms for the model variation problem and introduces and explores the link between model delivery sequences and balanced words. He also shows that the extended problem (obtained by including the suppliers' capacity constraints into the model) is NP-hard in the strong sense, and reviews algorithms for the extended problem. Finally he addresses the problem of minimizing the number of setups in delivery feasible supplier production sequences.

In Chapter 7, Marcotte and Savard present an overview of two classes of bilevel programs and their relationship to well-known combinatorial optimization problems, in particular the traveling salesman problem. In a bilevel program, a subset of variables is constrained to lie in the optimal set of an auxiliary mathematical program. Bilevel programs are hard to

solve, because they are generically non-convex and non-differentiable. Thus research on bilevel programs has followed two main avenues, the continuous approach and the combinatorial approach. The combinatorial approach aims to develop algorithms providing a guarantee of global optimality. The authors consider two classes of programs amenable to this approach, that is, the bilevel programs with linear or bilinear objectives.

In Chapter 8, Shepherd and Vetta present a study of *dijoins*. Given a directed graph $G = (V, A)$, a *dijoin* is a set of arcs B such that the graph $(V, A \cup B)$ is strongly connected. Shepherd and Vetta give two results that help to visualize *dijoins*. They give a simple description of Frank's primal-dual algorithm for finding a minimum *dijoin*. Then they consider weighted packings of *dijoins*, that is, multisets of *dijoins* such that the number of *dijoins* containing a given arc is at most the weight of the arc. Specifically, they study the cardinality of a weighted packing of *dijoins* in graphs for which the minimum weight of a directed cut is at least a constant k , and relate this problem to the concept of *skew submodular flow polyhedron*.

In Chapter 9, de Werra generalizes a coloring property of unimodular hypergraphs. A hypergraph H is *unimodular* if its edge-node incidence matrix is totally unimodular. A k -coloring of H is a partition of its node set X into subsets S_1, S_2, \dots, S_k such that no S_i contains an edge E with $|E| \geq 2$. The new version of the coloring property implies that a unimodular hypergraph has an equitable k -coloring satisfying additional constraints. The author also gives an adaptation of this result to balanced hypergraphs.

Acknowledgements The Editors are very grateful to the authors for contributing to this volume and responding to their comments in a timely fashion. They also wish to thank Nicole Paradis, Francine Benoît and André Montpetit for their expert editing of this volume.

DAVID AVIS
ALAIN HERTZ
ODILE MARCOTTE

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Chapter 1

VARIABLE NEIGHBORHOOD SEARCH FOR EXTREMAL GRAPHS. XI. BOUNDS ON ALGEBRAIC CONNECTIVITY

Slim Belhaiza

Nair Maria Maia de Abreu

Pierre Hansen

Carla Silva Oliveira

Abstract The algebraic connectivity $a(G)$ of a graph $G = (V, E)$ is the second smallest eigenvalue of its Laplacian matrix. Using the AutoGraphiX (AGX) system, extremal graphs for algebraic connectivity of G in function of its order $n = |V|$ and size $m = |E|$ are studied. Several conjectures on the structure of those graphs, and implied bounds on the algebraic connectivity, are obtained. Some of them are proved, e.g., if $G \neq K_n$

$$a(G) \leq \lfloor -1 + \sqrt{1 + 2m} \rfloor$$

which is sharp for all $m \geq 2$.

1. Introduction

Computers are increasingly used in graph theory. Determining the numerical value of graph invariants has been done extensively since the fifties of last century. Many further tasks have since been explored. Specialized programs helped, often through enumeration of specific families of graphs or subgraphs, to prove important theorems. The prominent example is, of course, the Four-color Theorem (Appel and Haken, 1977a,b, 1989; Robertson et al., 1997). General programs for graph enumeration, susceptible to take into account a variety of constraints and exploit symmetry, were also developed (see, e.g., McKay, 1990, 1998). An interactive approach to graph generation, display, modification and study through many parameters has been pioneered in the system Graph of Cvetković and Kraus (1983), Cvetković et al. (1981), and Cvetković and

Simić (1994) which led to numerous research papers. Several systems for obtaining conjectures in an automated or computer-assisted way have been proposed (see, e.g., Hansen, 2002, for a recent survey). The Auto-Graphix (AGX) system, developed at GERAD, Montréal since 1997 (see, e.g., Caporossi and Hansen, 2000, 2004) is designed to address the following tasks: (a) Find a graph satisfying given constraints; (b) Find optimal or near-optimal values for a graph invariant subject to constraints; (c) Refute conjectures (or repair them); (d) Suggest conjectures (or sharpen existing ones); (e) Suggest lines of proof.

The basic idea is to address all those tasks through heuristic search of one or a family of extremal graphs. This can be done in a unified way, i.e., for any formula on one or several invariants and subject to constraints, with the Variable Neighborhood Search (VNS) metaheuristic of Mladenović and Hansen (1997) and Hansen and Mladenović (2001). Given a formula, VNS first searches a local minimum on the family of graphs with possibly some parameters fixed such as the number of vertices n or the number of edges m . This is done by making elementary changes in a greedy way (i.e., decreasing most the objective, in case of minimization) on a given initial graph: rotation of an edge (changing one of its endpoints), removal or addition of one edge, short-cut (i.e., replacing a 2-path by a single edge) detour (the reverse of the previous operation), insertion or removal of a vertex and the like. Once a local minimum is reached, the corresponding graph is perturbed increasingly, by choosing at random another graph in a farther and farther neighborhood. A descent is then performed from this perturbed graph. Three cases may occur: (i) one gets back to the unperturbed local optimum, or (ii) one gets to a new local optimum with an equal or worse value than the unperturbed one, in which case one moves to the next neighborhood, or (iii) one gets to a new local optimum with a better value than the unperturbed one, in which case one recenters the search there. The neighborhoods for perturbation are usually nested and obtained from the unperturbed graph by addition, removal or moving of $1, 2, \dots, k$ edges.

Refuting conjectures given in inequality form, i.e., $i_1(G) \leq i_2(G)$ where i_1 and i_2 are invariants, is done by minimizing the difference between right and left hand sides; a graph with a negative value then refutes the conjectures. Obtaining new conjectures is done from values of invariants for a family of (presumably) extremal graphs depending on some parameter(s) (usually n and/or m). Three ways are used (Caporossi and Hansen, 2004): (i) a *numerical way*, which exploits the mathematics of Principal Component Analysis to find a basis of affine relations between graph invariants satisfied by those extremal graphs considered; (ii) a *geometric way*, i.e., finding with a “gift-wrapping” algorithm the

convex hull of the set of points corresponding to the extremal graph in invariants space: each facet then gives a linear inequality; (iii) an *algebraic way*, which consists in determining the class to which all extremal graphs belong, if there is one (often it is a simple one such as paths, stars, complete graphs, etc); then formulae giving the value of individual invariants in function of n and/or m are combined. Obtaining possible lines of proof is done by checking if one or just a few of the elementary changes always suffice to get the extremal graphs found; if so, one can try to show that it is possible to apply such changes to any graph of the class under study.

Recall that the Laplacian matrix $L(G)$ of a graph $G = (V, E)$ is the difference of a diagonal matrix with values equal to the degrees of vertices of G , and the adjacency matrix of G . The algebraic connectivity of G is the second smallest eigenvalue of the Laplacian matrix (Fiedler, 1973). In this paper, we apply AGX to get structural conjectures for graphs with minimum and maximum algebraic connectivity given their order $n = |V|$ and size $m = |E|$, as well as implied bounds on the algebraic connectivity.

The paper is organized as follows. Definitions, notation and basic results on algebraic connectivity are recalled in the next section. Graphs with minimum algebraic connectivity are studied in Section 3; it is conjectured that they are path-complete graphs (Harary, 1962; Soltès, 1991); a lower bound on $a(G)$ is proved for one family of such graphs. Graphs with maximum algebraic connectivity are studied in Section 4. Extremal graphs are shown to be complements of disjoint triangles, paths P_3 , edges K_2 and isolated vertices K_1 . A best possible upper bound on $a(G)$ in function of m is then found and proved.

2. Definitions and basic results concerning algebraic connectivity

Consider again a graph $G = (V(G), E(G))$ such that $V(G)$ is the set of vertices with cardinality n and $E(G)$ is the set of edges with cardinality m . Each $e \in E(G)$ is represented by $e_{ij} = \{v_i, v_j\}$ and in this case, we say that v_i is *adjacent* to v_j . The *adjacency matrix* $A = [a_{ij}]$ is an $n \times n$ matrix such that $a_{ij} = 1$, when v_i and v_j are adjacent and $a_{ij} = 0$, otherwise. The *degree* of v_i , denoted $d(v_i)$, is the number of edges incident with v_i . The *maximum degree* of G , $\Delta(G)$, is the largest vertex degrees of G . The *minimum degree* of G , $\delta(G)$, is defined analogously. The *vertex (or edge) connectivity* of G , $\kappa(G)$ (or $\kappa'(G)$) is the minimum number of vertices (or edges) whose removal from G results in a disconnected graph or a trivial one. A *path* from v to w