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Variable neighborhood search for extremal graphs. 16. Some conjectures related to the largest eigenvalue of a graph

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Abstract

We consider four conjectures related to the largest eigenvalue of (the adjacency matrix of) a graph (i.e., to the index of the graph). Three of them have been formulated after some experiments with the programming system AutoGraphiX, designed for finding extremal graphs with respect to given properties by the use of variable neighborhood search. The conjectures are related to the maximal value of the irregularity and spectral spread in *n*-vertex graphs, to a Nordhaus–Gaddum type upper bound for the index, and to the maximal value of the index for graphs with given numbers of vertices and edges. None of the conjectures has been resolved so far. We present partial results and provide some indications that the conjectures are very hard.

Keywords: Graph; Adjacency matrix; Largest eigenvalue; Index; Spectral spread; Irregularity; Variable neighborhood search; Extremal graph; Conjectures; AutoGraphiX

1. Introduction

Variable neighborhood search (VNS) (Hansen and Mladenović, 2001; Mladenović and Hansen, 1997) appears to play a specific role in the connections and interactions between combinatorial optimization and extremal graph theory.

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Combinatorial optimization (Mathematics Subject Classification: 90C27) deals with solving optimization problems of the following type:

$$\min_{x \in S} f(x), \tag{1}$$

where S is a finite or infinite denumerable set and $f : S \to \mathbb{R}$. In most cases the set of feasible solutions S is a finite set.

Extremal graph theory (Mathematics Subject Classification: 05C35) deals with finding (lower and/or upper) bounds for various graph invariants under some constraints imposed on other graph invariants (Bollobás, 1978, 1995). The construction of extremal graphs, i.e., graphs meeting these bounds is a natural part of such investigations.

The key observation of Cvetković et al. (2004) is that the uniting feature of these two disciplines is the fact that both deal with problems of finding extrema of a real function defined on a finite set.

There are many problems in (extremal) graph theory where one looks for extrema of a graph invariant for graphs with a fixed number of vertices. Such a problem can be represented in the form of (1) where S is the set of all (or some) graphs on a fixed number of vertices and for a graph $x \in S$ the function $f(x)$ is a graph invariant. Such a problem was recognized as a generic problem of combinatorial optimization for the first time in Caporossi and Hansen (2000).

A computer program called AutoGraphiX (AGX), for finding extremal (or near-extremal) graphs with respect to some properties, has been described in Caporossi and Hansen (2000). The paper was just the beginning of a series of papers in which results obtained by AGX are presented. To this series belong the papers Caporossi and Hansen (2000), Caporossi et al., 1999, Cvetković et al., 2001, 1999, Caporossi and Hansen, 2004, Hansen and Mélot, 2003, 2005, Fowler et al., 2001, Aouchiche et al., 2001, Gutman et al., 2005, Aouchiche et al., 2005, Aouchiche and Hansen, 2005, Belhaiza et al., 2005, Hansen et al., 2005, Hansen and Stevanović, 2005 (and this paper as well).

As one of the first test examples, the following extremal problem with previously known solution was tested by AGX (cf. Caporossi and Hansen, 2000). Let $\mathscr{T}_n$ be the set of trees on n vertices and let $\lambda_1(G)$ be the largest eigenvalue of the adjacency matrix of a graph G. Find

$$\min_{T \in \mathscr{T}_n} \lambda_1(T), \quad \max_{T \in \mathscr{T}_n} \lambda_1(T) \tag{2}$$

and the corresponding extremal trees. As is well known, the minimum is attained for a path P_n with $\lambda_1(P_n) = 2\cos\frac{\pi}{n+1}$ and the maximum for a star $K_{1,n-1}$ with $\lambda_1(K_{1,n-1}) = \sqrt{n-1}$ (cf. Lovász and Pelikan, 1973). The system AGX has successfully found these extremal trees for several values of n (cf. Caporossi and Hansen, 2000). Obviously, problems (2) are of the form (1).

Combinatorial optimization and extremal graph theory existed for many years without notable interactions. For example, the books (Bollobás, 1978, 1995) on extremal graph theory do not refer to combinatorial optimization.

Recently, the idea was built into the system AGX (Caporossi and Hansen, 2000) and the application of this system to actual research on extremal problems in graph theory clearly indicates a possibility of connecting the two fields. Some general solving procedures of combinatorial optimization can be used via programming systems, such as AGX, to solve problems of extremal graph theory in order to give hints concerning theoretical considerations. In particular, variable neighborhood search is used as the main (meta-)heuristic within the system AGX.

For example, in Cvetković et al. (2001) the system AGX has found extremal spanning trees of a complete bipartite graph $K_{m,n}$ for various m and n w.r.t. the objective function $\lambda_1(T)$. Many conjectures arose and some of them have been proved in Cvetković et al. (2001).

Since this early work, AGX has been developed along several lines. Three ways to automate conjecture making were outlined in Caporossi and Hansen (2004): (i) a numerical method which is applied to vectors of values of invariants for the extremal graphs found, and which uses the mathematics of Principle Component Analysis to find a basis of affine relations between graph invariants; (ii) a geometric method which considers extremal graphs as points in invariant space and uses a gift-wrapping algorithm to determine their convex hull, facets of which correspond to inequality relations; (iii) an algebraic method which recognizes