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ON SOME INTERCONNECTIONS BETWEEN COMBINATORIAL OPTIMIZATION AND EXTREMAL GRAPH THEORY

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The uniting feature of combinatorial optimization and extremal graph theory is that in both areas one should find extrema of a function defined in most cases on a finite set. While in combinatorial optimization the point is in developing efficient algorithms and heuristics for solving specified types of problems, the extremal graph theory deals with finding bounds for various graph invariants under some constraints and with constructing extremal graphs. We analyze by examples some interconnections and interactions of the two theories and propose some conclusions.

Keywords: Combinatorial optimization, extremal graph theory, variable neighborhood search, mathematical programming.

1. INTRODUCTION

We list a few details from Mathematics Subject Classification 2000 which are relevant for our discussion.

05 Combinatorics
05C Graph Theory
05C35 Extremal Problems
05C90 Graph Algorithms

90 Operations Research, Mathematical Programming
90C Mathematical Programming
90C27 Combinatorial Optimization
90C35 Programming Involving Graphs and Networks
90C22 Semidefinite Programming

68 Computer Science
68R Discrete Mathematics in Relation to Computer Science
68R10 Graph Theory
68W Algorithms
68W05 Non-numerical Algorithms

We shal discuss some relations between *combinatoral optimization* (90C27) and *extremal problems in graph theory* or *extremal graph theory* (05C35). Some related fields from Mathematic Subject Classification 2000 are given as well.

Combinatorial optimization (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 $f : S \to R$. In most cases the set of feasible solutions S is a finite set.

Extremal graph theory (05C35) deals with finding (lower and/or upper) bounds for various graph invariants under some constraints imposed on other graph invariants [3], [4]. Construction of extremal graphs, i.e. graphs meeting these bounds is a natural part of such investigations.

Our key observation 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. We shall support this assertion by several examples.

Typical problems of combinatorial optimization are integer programming and optimization problems defined on weighted graphs.

In integer programming the set S of feasible solutions is the set of points with integer coordinates in a convex polyhedron in R^n which is defined by some (linear) constraints. Usually, the set is finite and in the case that it is infinite and the task has a solution, one can impose some further constraints to make S finite without changing the solution.

As an example of the second group, consider the task of finding a shortest path between two vertices in a (finite) weighted graph. The set of feasible solutions S is the set of all paths between the specified vertices and it is infinite if we allow paths to go several times through a vertex. However, S becomes finite if we consider simple paths (which is usually done since a shortest path is always simple).

There are many problems in (extremal) graph theory where one looks for extrema of a graph invariant for graphs with the fixed number of vertices. Such a problem can be represented in the form (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. As far as we know, such a problem is recognized as a problem of combinatorial optimization in [7] for the first time.

A computer program, called AutoGraphiX (AGX), for finding extremal graphs with respect to some properties has been described in [7]. The paper was just the beginning of a series of papers in which results obtained by AGX are being presented. To this series belong the papers [7, 5, 11, 6, 8, 15, 9, 1, 16, 14].

As one of the first testing examples, the following extremal problem (with previously known solution) was tested by AGX (cf. [7]). Let $\mathcal{T}_n$ 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

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

and the corresponding extremal trees. As it is well known, minimum is attained for a path P_n with $\lambda_1(P_n) = 2\cos\dfrac{\pi}{n+1}$ and the maximum for a star $K_{1,n-1}$ with $\lambda_1(K_{1,n-1}) = \sqrt{n-1}$ (cf. [18]). Obviously, problems (2) are of the form (1).

The next example is the famous Turán problem [23], the "first" one in the extremal graph theory, given here for simplicity in a special case.

Let $\mathcal{G}_n^{(wt)}$ be the set of graphs on n vertices without triangles and let $m(G)$ be the number of edges of a graph G. Find

$$\max_{G \in \mathcal{G}_n^{(wt)}} m(G) \tag{3}$$

and the corresponding extremal graphs. The solution is well known: maximal number of edges is $[n^2/4]$ and the only extremal graph is the complete bipartite graph $K_{p,p}$ for $n = 2p$ and $K_{p,p-1}$ for $n = 2p+1$. Again (3) is of the form (1).

We mention also the following two related recent results.

Since $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ contains no odd cycles, the maximal number of edges in a graph containing no C_{2k+1} is $\lfloor n^2/4 \rfloor$ for sufficiently large n. The main aim of the paper [2] is to prove a considerable strenghtening of this result. Let us write $f(n, \Delta, C_{2k+1})$ for the maximal number of edges in a graph of order n and maximum degree Δ that contains no cycles of length $2k+1$. For $n/2 \le \Delta \le n-k-1$ and n sufficiently large it is shown that $f(n, \Delta, C_{2k+1}) = \Delta(n-\Delta)$, with the unique extremal graph being a complete bipartite graph.

The 2-stability number $\alpha_2(G)$ of a graph G is the maximum order of a bipartite induced subgraph of G. A lower bound on $m = |E(G)|$ is given as a function of $n = |V(G)|$ and $k = \alpha_2(G)$. Minimal graphs are also described as disjoint unions of balanced cliques and isolated vertices [13].

According to [4], in a typical extremal problem, given a property $\mathcal{P}$ and an invariant Φ for a class $\mathcal{S}$ of graphs, we wish to determine the least value f for which every graph G in $\mathcal{S}$ with $\Phi(G) > f$ has property $\mathcal{P}$. The graphs in $\mathcal{S}$ without property $\mathcal{P}$ and satisfying $\Phi(G) = f$ are the *extremal graphs* for the problem. More often than not, $\mathcal{S}$ consists of graphs of the same order n, namely $\mathcal{S} = \{G \in \mathcal{H} : |G| = n\}$, where $\mathcal{H}$ is a class of graphs, and so f is considered to be a function of n, determined by Φ and $\mathcal{H}$. This function $f(n)$ is the *extremal function* for the problem.

Obviously, this problem can be reformulated in the form (1) in the following way

$$f = \max_{G \in \mathcal{S}_{\neg\mathcal{P}}} \Phi(G) \tag{4}$$

where $\mathcal{S}_{\neg\mathcal{P}}$ is the set of graphs from $\mathcal{S}$ which do not have property $\mathcal{P}$.

Also, any problem of the form (1) can be converted into the above described form typical for extremal graph theory. For example, the second problem (2) can be stated as the problem of finding the least value f such that $\lambda_1(G) > f$ implies that the graph G contains a cycle (i.e. is not a tree).

2. DIFFERENT APPROACHES AND GOALS

The main objective in combinatorial optimization is to develop efficient algorithms and heuristics for solving various *types* of problems of the form (1). For each problem type we have a set of instances. No solutions are known in advance. For each instance a solving procedure (an algorithm or a heuristics) should be executed and a solution found in this way.

Extremal graph theory deals with solving and solutions by theoretical means of various *concrete* problems of the form (1). The set S of feasible solutions is usually a set of graphs with a fixed number of vertices. Typical results are: finding a bound for the objective function, showing that the bound is tight by constructing a graph which attains the bound, and constructing or characterizing extremal graphs. The algortihmic complexity of constructing procedures is usually not the subject of considerations.

3. POSSIBLE INTERACTIONS BETWEEN THE TWO FIELDS

Combinatorial optimization and extremal graph theory existed for many years without notable interactions. For example, books [3, 4] on extremal graph theory do not refer to combinatorial optimization.

Recently, the idea built into the system AGX [7] and the application of this system to actual research on extremal problems in graph theory clearly indicate a possibility to connect the two fields. Some general solving procedures of combinatorial optimization can be used via the programming systems, such as AGX, to solve the problems of extremal graph theory in order to give hints to theoretical considerations.

For example, in [11] the system AGX has found extremal spanning trees of a complete bipartite graph $K_{m,n}$ for various m and n with respect to the objective function $\lambda_1(T)$. Many conjectures arose and some of them have been proved in [11].

Posing conjectures by the aid of a system like AGX is a two step procedure. In the first step one estimates the values of the extremal function $f = f(n)$ for a problem of a type (4) for several appropriate values of n by finding an extremal or a nearly extremal graph. On the basis of the values obtained in the first step one tries to find a general expression for $f(n)$. This second step can be done by the user but also the system AGX can do this under some circumstances in several ways [8]. It is not important that there is no warranty that the graphs obtained by AGX are really extremal. Anyway, the conjecture has to be proved by theoretical means. It is nonsignificant whether a disproved conjecture is false because the statements were wrong in the first or in the second step of the conjecture posing process.

Although the problems of extremal graph theory are of the general type (1) typical for combinatorial optimization, their concrete forms are various and, as a rule, such that there are no known algorithms in combinatorial optimization for solving them. Therefore, some general heuristics, like those known as meta-heuristics, need to be applied. Just such an approach has been adopted in creating the system AGX. The meta-heuristics called Variable Neighborhood Search (VNS) has been selected [21], [17].

An alternative to heuristic search for extremal graphs is to use exhaustive search. Such an approach has been used in many cases (for example, by the use of system GRAPH [10, 22] for modest sizes of graph sets and by Nauty for extensive searches [19, 20]). However, due to the enormous number of graphs an extensive search over all graphs is (nowadays) possible for graphs up to 11 or 12 vertices. A heuristic approach enables, however, to find extremal or nearly extremal graphs with up to 30 vertices, although a warranty that they are really extremal is missing without further theoretical considerations.

Other general tools of combinatorial optimization can be applied to the extremal graph theory at least in principle. First of all, the problems of extremal graph theory can be represented as integer programming problems. For example, the Turán problem (3) can be formulated as the problem

$$\max \sum_{i=1}^{n} \sum_{j=1}^{n} x_{ij}$$

where $x_{ij} = x_{ji}$, $x_{ii} = 0$, $x_{ij} \in \{0,1\}$ $(i, j = 1,2,...,n)$ and $x_{ij} + x_{jk} + x_{ki} \le 2$ for distinct $i, j, k = 1,2,...,n$. Although solving extremal graph problems in this way looks questionable, some theorems of integer programming could perhaps give some useful hints as how to treat the problems.

Semidefinite programming can be also used in some situations, especially in problems involving eigenvalues.

For a symmetric matrix X we write $X \geq 0$ to denote that it is positive-semidefinite. For a given symmetric matrix, the largest eigenvalue λ_1 can be obtained by a semidefinite programming task

$$\lambda_1 = \min_{\substack{t \in R \\ tI - X \geq 0}} t$$

while the first of problems (2) can be converted to the form

$$\lambda_1 = \min_{\substack{(x,t) \in \mathcal{X}_n \times R \\ tI - X \geq 0}} t$$

where $\mathcal{X}_n$ is the set of adjacency matrices of trees on n vertices which is determined in a standard way: 0-1 variables, zero-diagonal, a fixed sum of entries and, to ensure the connectedness, the constraints similar to the well-known sub-tour elimination constraints in the traveling salesman problem.

An alternative to the use of adjacency matrices, in general and in treating problems of extremal graph theory by semidfinite programming, is to introduce the Laplacian matrix. Then the graph connectedness condition, very often appearing in extremal graph problems, can be suitably imposed using the concept of the algebraic connectivity of a graph (the second smallest eigenvalue of the Laplacian matrix) as already used in the traveling salesman problem [9].

In the other direction, the influence of extremal graph theory to combinatorial optimization is also possible. The extremal graph theory offers a variety of combinatorial optimization problems of type (1) for whose solutions no specific algorithms or heuristics exist. It would be a challenge to develop efficient solving procedures for some of such problems with unknown solutions.

Combinatorial optimization problems coming from extremal graph theory have a specific form regarding the set of instances. An instance is a set of graphs specified by the number of vertices and by other graph invariants, i.e. the set of instances is a set of sets of graphs. The instance is identical with the set of feasible solutions.

We can imagine that the graphs on n vertices forming an instance are sub-graphs of a complete graph K_n. In this artificial way the instances would be simply complete graphs with conditions defining the actual set of subgraphs. Now we would have some similarities with optimization problems defined on weighted graphs which appear in combinatorial optimization.

A relaxation of such a problem would mean an extension of the instance to a broader class of graphs or even to objects which are not graphs. The later case occurs, for example, if we represent the graphs from an instance by their adjacency matrices and then formulate a relaxation task by looking for the extremum over all (not necessarily 0-1) matrices.

One can think of possibilities of constructing branch and bound algorithms for problems of extremal graph theory which would accelerate an exhaustive search and, of course, would really provide extremal graphs. A way to realize branching rules in such algorithms would be to introduce penalty terms for some graph invariants into the objective function in order to ensure the presence of the desired class of graphs in new relaxation tasks.

The strategy for solving a problem of above type depends also on the character of the objective function. It could be "continuous" in the sense that the set of its values over all graphs is everywhere dense at least in some intervals (e.g. $\lambda_1(G)$). This means that local modifications of graphs which appear, for example in VNS, can be arranged so that they cause small changes of the objective function.

The other situation appears in the discrete case where, for example, the objective function has integer values (e.g. $m(G)$). An idea to overcome this situation is to look at the relaxation with general matrices and to express the objective function through matrix parameters (e.g. entries, eigenvalues, etc.).

4. CONCLUSIONS

This paper elaborates mutual connections and differences between combinatorial optimization and extremal graph theory. Our key observation 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. This observation enables using general combinatorial optimization procedures in treating problems in extremal graph theory. In particular, some examples of using combinatorial optimization tools to generate conjectures in extremal graph theory are described.

REFERENCES

[1] Aouchiche, M., Caporossi, G., and Hansen, P., "Variable Neighborhood Search for extremal graphs, 8. Variations on Graffiti 105", *Cong. Numer.*, 148 (2001) 129-144.

[2] Balister, P., Bollobás, B., Riordan, O., and Schelp, R.H., "Graphs with large maximum degree containing no odd cycles of a given length", *J. Combin. Theory Ser. B*, 87 (2) (2003) 366-373.

[3] Bollobás, B., *Extremal Graph Theory,* Academic Press, London-New York-San Francisco, 1978.

[4] Bollobás, B., "Extremal graph theory", in: R.L. Graham, M.Grötschel, L.Lovász, (eds.), *Handbook of Combinatorics I, II,* Elsevier-Amsterdam, MIT Press-Cambridge, MA, 1995, 1231-1292.

[5] Caporossi, G., Cvetković, D., Gutman, I., and Hansen, P., "Variable Neighborhood Search for extremal graphs, 2. Finding graphs with extremal energy", *J. Chem. Inf. Comp. Sci.*, 39 (1999) 984-996.

[6] Caporossi, G., Gutman, I., and Hansen, P., "Variable Neighborhood Search for extremal graphs, 4. Chemical trees with extremal connectivity index", *Comput. Chem.*, 23 (1999) 469-477.

[7] Caporossi, G., and Hansen, P., "Variable Neighborhood Search for extremal graphs I", *Discrete Math.*, 212 (2000) 29-44.

[8] Caporossi, G., and Hansen, P., "Variable Neighborhood Search for extremal graphs, 5. Three ways to automate finding conjectures", *Discrete Math.*, 276 (2004) 81-94.

[9] Cvetković, D., Čangalović, M., and Kovačević-Vujčić, V., "Semidefinite programming methods for the symmetric travelling salesman problem", in: G. Cornnejols, R.E. Burkard, G.J. Woeginger (eds.), *Integer Programming and Combinatorial Optimization, Proc. 7th Int. IPCO Conf., Graz, Austria, June 1999,* Lecture Notes Comp. Sci. 1610, Springer, Berlin, 1999, 126-136.

[10] Cvetković, D., and Simić, S., "Graph theoretical results obtained by the support of the expert system "Graph"", *Bull. Acad. Serbe Sci. Arts, Cl. Sci. Math. Natur., Sci. Math.*, 107 (19) (1994) 19-41.

[11] Cvetković, D., Simić, S., Caporossi, G., and Hansen, P., "Variable Neighborhood Search for extremal graphs, 3. On the largest eigenvalue of color-constrained trees", *Linear and Multilinear Algebra*, 49 (2001) 143-160.

[12] Fowler, P.W., Hansen, P., Caporossi, G., and Sondini, A., "Variable Neighborhood Search for extremal graphs, 7. Polyenes with maximum HOMO-LUMO gap", *Chem. Phys. Letters*, 49 (2001) 143-146.

[13] Gerber, M.U., Hansen, P., and Hertz, A., "Extensions of Turán's theorem to the 2-stability number", *Graphs Combin.,* 18 (3) (2002) 479-489.

[14] Gutman, I., Hansen, P., and Mélot, H., "Variable Neighborhood Search for extremal graphs, 10. Comparison of irregularity indices for chemical trees", to appear.

[15] Hansen, P., and Mélot, H., "Variable Neighborhood Search for extremal graphs, 6. Analyzing bounds for the connectivity index", *J. Chem. Inform. Comput. Sci.*, 43 (2003) 1-14.

[16] Hansen, P., and Mélot, H., "Variable Neighborhood Search for extremal graphs, 9. Bounding irregularity of a graph", to appear.

[17] Hansen, P., and Mladenović, N., "Variable Neighborhood Search: Principles and applications", *EJOR*, 130 (2001) 449-467.

[18] Lovász, L., and Pelikan, S., "On the eigenvalues of trees", *Periodica Math. Hung*., 3 (1-2) (1973) 175-182.

[19] McKay, B.D., "Nauty user's guide (version 1.5)", Technical Report, TR-CS-90-02, Department of Computer Science, Australian National University, 1990.

[20] McKay, B.D., "Isomorph-free exhaustive generation", *J. Algorithms*, 26 (1998) 306-324.

[21] Mladenović, N., and Hansen, P., "Variable Neighborhood Search", *Comp. Oper. Res*., 24 (1997) 1097-1100.

[22] Petrović, R., Guberinić, S., Batanović, V., and Cvetković, D., "Operational research models in action, the result of international cooperation, a potpourri", *EJOR*, 87 (1995) 500-506.

[23] Turán, P., "Eine extremalaufgabe aus der graphentheorie", *Fiz. Mat. Lapok*, 48 (1941) 436-452.