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## On bags and bugs $\stackrel{\text{tr}}{\sim}$

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## Abstract

Usual graph classes, such as complete graphs, paths, cycles and stars, frequently appear as extremal graphs in graph theory problems. Here we want to turn the reader's attention to two novel, simply defined, graph classes that appear as extremal graphs in several graph theory problems. We call them bags and bugs. As examples of problems where bags and bugs appear, we show that balanced bugs maximize the index of graphs with fixed number of vertices and diameter  $\ge 2$ , while odd bags maximize the index of graphs with fixed number of vertices and radius  $\ge 3$ .

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## 1. Introduction

Graph theory deals extensively with graph invariants, i.e., functions  $i_G$  of the set of all graphs G (or a subset thereof, such as all connected graphs) into the reals or the integers (and usually taking only positive values). There are many well-known invariants, such as the independence and chromatic numbers, the radius and diameter and the index (the largest eigenvalue of G's adjacency matrix). Extremal graph theory [2] deals with the problem of characterizing the families of graphs G for which an invariant  $i_G$  is minimum or maximum.

Recently, it has been observed in [5,6,9] that this problem can be viewed as one of parametric combinatorial optimization and, moreover, that a *generic* heuristic can be used to solve it, for any invariant or formula defined on one or several invariants which is readily computable. Using the variable neighborhood search metaheuristic [11], this idea has been implemented in the system *AutoGraphiX*. It yields, among other results, conjectures on the structure of extremal graphs. Extensive use of that system has shown that the families of extremal graphs for given invariants, as well as for sums, differences, ratios or products of two invariants, are often well-known simple ones, e.g., paths, stars, cycles, complete graphs, complete bipartite graphs and complete split graphs. Several apparently novel families

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Fig. 1. An odd *Bag*<sub>5,5</sub> and a *Bug*<sub>5,3,3</sub>.

have also been observed. In this paper, we discuss two of them, which we call bags and bugs. They are defined as follows:

**Definition 1.** A bag  $Bag_{p,q}$  is a graph obtained from a complete graph  $K_p$  by replacing an edge uv with a path  $P_q$ . A bag is odd if q is odd, otherwise it is even.

So, in  $Bag_{p,q}$  the number of vertices is n = p + q - 2 and the number of edges is  $m = \binom{p}{2} + q - 2$ .

**Definition 2.** A bug  $Bug_{p,q_1,q_2}$  is a graph obtained from a complete graph  $K_p$  by deleting an edge uv and attaching paths  $P_{q_1}$  and  $P_{q_2}$  at u and v, respectively. A bug is balanced if  $|q_1 - q_2| \leq 1$ .

So, in  $Bug_{p,q_1,q_2}$  the number of vertices is  $n = p + q_1 + q_2 - 2$  and the number of edges is  $m = \binom{p}{2} + q_1 + q_2 - 3$ . Fig. 1 gives examples of a bag and a bug.

Let G = (V, E) be a simple connected graph. *Eccentricity* of a vertex  $v \in V$  is the maximum distance from v to any other vertex of G. Then, the *diameter* is the maximum, while the *radius* is the minimum among eccentricities of all vertices of G. Denote the adjacency matrix of G by A(G). The polynomial  $P_G(\lambda) = \det(\lambda I - A(G))$  is called the *characteristic polynomial* of G, while its roots, the eigenvalues of A(G), are called eigenvalues of G. The largest eigenvalue  $\lambda_1(G)$  of G is called its *index*. For other undefined notions, see [1,7].

From the Perron–Frobenius theory of nonnegative matrices it follows that  $\lambda_1(G)$  has a positive eigenvector *x* satisfying the *eigenvalue equation* 

$$A(G)x = \lambda_1(G)x.$$

The index of G can also be characterized by a Rayleigh quotient

$$\lambda_1(G) = \sup_{y \neq 0} \frac{y^{\mathrm{T}} A(G) y}{y^{\mathrm{T}} y}$$

where the supremum is attained for an eigenvector *x* of  $\lambda_1(G)$ .

The following problem concerning the index of graphs was proposed by Brualdi and Solheid [4]: Given a set S of graphs, find an upper bound for the index of graphs in S and characterize the graphs for which this bound is attained. The cases when S is the set of all graphs or of all trees are considered classics in the literature on spectral graph theory

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