MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **58** (2007) 365-384

ISSN 0340 - 6253

Variable Neighborhood Search for Extremal Graphs. 20. Automated Comparison of Graph Invariants

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(Received June 28, 2006)

Abstract

A graph invariant is a function of a graph G which does not depend on labeling of G's vertices or edges. An algebraic expression of one or several graph invariants is itself an invariant. Graph theory is replete with theorems about graph invariants, which are either algebraic, *i.e.,* equalities or inequalities involving such invariants, or structural, *i.e.,* characterizations of which families of graphs are extremal for a given invariant, that is give it maximum or minimum value. Both types of results can be conjectured by the system AutoGraphiX 2 (AGX 2), in an automated way, or, in some carefully distinguished cases, in an assisted way. We report here on a systematic comparison of 20 graph invariants: for each pair of them, AGX 2 considers the four operations $+, -, \times, /$ and derives best possible lower and upper bounding functions of the number of vertices, as well as extremal graphs. Out of 1520 cases, AGX 2 recognizes 37 known results, derives automatically algebraic and corresponding structural conjectures in 1260 cases (841 of which are proved automatically), and structural conjectures only in 168 more cases, from which algebraic conjectures could be derived by hand in 86 cases. No results were obtained in 55 cases. Manual or assisted proofs have been obtained in 394 cases, 22 conjectures were refuted and 171 conjectures remain open. Many examples are given. AGX 2 is also compared to the three operational systems GRAPH, GRAFFITI and HR.

1 Introduction

Computers have long been used in applications of graph theory to many fields, *e.g.* when solving some optimization problem defined on a graph. But the role of computers in graph theory [37] is not limited to applications. Indeed, computers can also be used to advance the theory *per se*, *i.e.,* to provide conjectures, refutations and proofs (or ideas of proofs).

While only a few attempts have been made at full automation of proofs in graph theory [23, 24, 28, 29, 30], partial automation of complex proofs has been fruitful. The prominent example is, of course, the 4-color theorem [6, 7, 8, 48]. Nowadays, computer help in proofs having an enumerative character is quite frequent; to illustrate a "dynamic survey" of small Ramsey numbers [46] cites 93 cases of computer use among 327 papers.

Much work has also been devoted to assisted, or in some rare cases, automated discovery of conjectures. Operational systems for that purpose (among others) are GRAPH [23, 24], GRAFFITI [26, 31, 32], AutoGraphiX (AGX) [3, 4, 16, 17] and HR [21]; some other systems such as GRAPH THEORIST [28, 29, 30], INGRID [12, 13, 14] and NAUTY [42] can also be helpful in that respect, see [38, 39] for review and discussions.

A graph invariant is a function of a graph G which does not depend on labeling of G's vertices or edges. Examples of graph invariants are the diameter, the radius, the average distance, the independence number and the index (definitions will be given below). Graph theory is replete with theorems involving graph invariants. They are either *algebraic*, *i.e.,* equalities or inequalities involving one or several invariants, or *structural*, *i.e.,* characterizations of the families of graphs for which an invariant takes an extremal value.

Both types of results can be conjectured by the system AGX, in a fully automated way, or in some cases, to be carefully distinguished, in an assisted way. This system has been developed at GERAD, Montreal, since about 10 years. Its principles, successive implementations and applications to numerous problems of graph theory and mathematical chemistry are described in a series of papers, to which the present paper also belongs. For references to other papers in this series see [4]. Recently, a new version of that program, called AGX 2 [3], has been developed and systematically tested, focusing on its functions for conjecture discovery and proof of easy propositions (AGX 2 can also be used for several other purposes, *e.g.* refuting, repairing or strengthening conjectures and finding ideas of proof for more difficult propositions or theorems). It is the purpose of the present paper to report on the results of these experiments. More precisely, we considered 20 invariants and sought expressions of the following form (called AGX Form 1):

$$\underline{b}(n) \leq i_1 \oplus i_2 \leq \overline{b}(n) \tag{1}$$

where i_1 and i_2 are invariants of a graph G from the chosen set of 20, $\oplus$ denotes one of the 4 operations $+, -, /$ and $\times$, $\underline{b}(n)$ and $\overline{b}(n)$ are, respectively, lower and upper bounding functions depending on the *order* n, or number of vertices, of G which are *best possible*, *i.e.,* such that

for each value of n (except possibly very small ones, due to border effects) there is a graph G for which the bound is tight. The order of invariants i_1 and i_2 in (1) is arbitrary. For $\oplus$ equal to $+$ or $\times$, changing this order has no effect; for $\oplus$ equal to $-$ or $/$, such a change permutes lower and upper bounds (bounds being multiplied by -1 in the former case and ratios in the bounds inversed also in the latter one). Note that the form (1) is reminiscent of the well-known Nordhaus-Gaddum relations [45]; however, it generalizes this last form in three ways:
(i) the operations $-$ and $/$ are considered in addition to $+$ and $\times$,
(ii) the invariants i_1 and i_2 are independent instead of having $i_2(G) = i_1(\overline{G})$, where $\overline{G}$ denotes the complementary graph of G, in which an edge joins vertices v_i and v_j if and only if there is no such edge in G,
(iii) it is mandatary that the lower and upper bounds be best possible (instead of this only being desirable).
Results for a pair of invariants can be *complete*, *i.e.,* consist of both conjectured best possible functions $\underline{b}(n)$ and $\overline{b}(n)$ and the corresponding characterizations of the extremal graphs, or *structural*, *i.e.,* consist of the characterizations of extremal graphs only. This last case occurs when algebraic expressions for $\underline{b}(n)$ and $\overline{b}(n)$ are too difficult for AGX 2 to obtain, or when such expressions do not exist, *e.g.* because they correspond to solutions of an equation of degree 5 or more.
In some fairly frequent cases, complete results are simple and can be proved by AGX 2 in a fully automated way; we then refer to them as *observations*. If results are structural, algebraic expressions for $\underline{b}(n)$ and $\overline{b}(n)$ can sometimes be deduced, in an assisted way, from the characterization of extremal graphs. In some fairly rare cases the graphs obtained by AGX 2 and conjectured to be extremal present very little or no regularity and no results are obtained.
The paper is organized as follows. The principle of AGX 2, *i.e.,* the way it applies to graph theory the Variable Neighborhood Search metaheuristic [40, 44], and the three ways it analyzes results to derive conjectures, are summarized in the next section. Experiments are discussed in Section 3. Results are reported, and illustrated by examples in Section 4. A comparison of AGX 2 with the three systems GRAPH, GRAFFITI and HR is made and illustrated by examples in Section 5. Brief conclusions are drawn in the last section.

2 Principles of AGX 2

Let $\mathcal{G}_n$ and $\mathcal{G}_{n,m}$ denote respectively the sets of all graphs with n vertices, and with n vertices and m edges. Two basic ideas underly the systems AGX 1 and AGX 2:
(i) *Most problems of extremal graph theory can be viewed as problems of parametric combinatorial optimization of the form*

$$\min / \max_{G \in \mathcal{G}_n} i(G) \quad \text{or} \quad \min / \max_{G \in \mathcal{G}_{n,m}} i(G) \tag{2}$$

for some invariant $i(G)$ with parameters n and m, or the exploitation of their solutions;
(ii) All problems of the form (2) can be solved approximately by a generic heuristic.
To obtain such a heuristic, the Variable Neighborhood Search metaheuristic (VNS) [40, 44], a general framework for building heuristics, is specialized. VNS exploits systematically changes in neighborhoods used in the search, both in a descent phase to obtain a locally extremal graph, and in a "shaking" phase, to get out of the corresponding valley (or away from the corresponding mountain) in order to find a better graph. Neighborhoods correspond to changes brought to the graph G, *e.g.* all ways to add, or to remove an edge, and so forth.
Rules of VNS applied in AGX 1 and AGX 2 are the following:

(0) Select the set of neighborhood structures $N_k,\ k = 1, \ldots k_{max}$ that will be used in the search for a better locally optimal graph, and a stopping condition. Choose an initial graph G.

Repeat until the stopping condition is met:

1. Set $k = 1$;

2. Until $k = k_{max}$, repeat the following steps:

   (a) (*shaking*) generate a graph G' from the k^{th} neighborhood of G $(G' \in N_k(G))$;

   (b) (*descent*) apply *Variable Neighborhood Descent (VND)* with G' as initial graph; denote with G'' the locally optimal graph obtained;

   (c) (*improvement or continuation*) if $i(G'')$ is better than $i(G)$, best value of i for a previously visited graph, move there, *i.e.,* replace G by G'', and continue search within $N_1(G)$; otherwise, set $k \leftarrow k + 1$.

The stopping condition is usually a maximum computing time. The VND routine is a descent one in which one considers in turn various transformations applied to G; if one is beneficial, G is modified accordingly; if not one proceeds to the next move (or neighborhood) until a local optimum for all moves is attained. In AGX 1 the moves considered were rotation of an edge, addition of an edge, removal of an edge, displacement of an edge (removal followed by addition), detour (replacing an edge by a path of two edges), short-cut (reverse of the previous move) and a few others. In AGX 2, all possible moves on 2 vertices, then on 3, then on 4 are considered in turn. Moreover, moves which have been useful at the beginning of the search are emphasized automatically, *i.e.,* applied more frequently than others.
Once a set of (presumably) extremal graphs has been found, bounding functions $\underline{b}(n)$ and $\overline{b}(n)$ are deduced by one of the following 3 approaches [17]:
(i) a *numerical method* [15] which applies the mathematics of Principle Component Analysis to determine, in polynomial time, a basis of affine relations between invariants, satisfied by the extremal graphs found. This method must be applied in a different way in the case of relations of AGX Form 1. Indeed one seeks nonlinear inequalities instead of linear equalities. Considering

minimum, or maximum values of $i_1 \oplus i_2$ for all n in the chosen range it reduces to fitting exactly to those points a function of the single variable n. This function is a linear combination of terms in n, n^2, $1/n$, $\sqrt{n-1}$ and possibly other similar terms which often appear in graph theory. If successful, this gives an analytical expression for $\underline{b}(n)$, or $\overline{b}(n)$. Numerous formulae are obtained in this way, as a true inequality of AGX Form 1 exists for all i_1, i_2 and $\oplus$. So the numerical method is far from being limited to the discovery of linear equalities, as erroneously stated in [41] page 311;
(*ii*) a *geometric method* which views extremal graphs as points in invariants space and applies a ″gift-wrapping″ algorithm to find their convex hull and linear inequality relations associated with its facets. Note that a similar approach is used in the recent system GraPHedron [18, 43];
(*iii*) an *algebraic method* [1, 3] which recognizes to which family (or families) of graphs the extremal graphs belong, then uses a database of formulae for invariants in function of the order of G to obtain bounding functions. After substitution of formulae for i_1 and i_2 in (1), simplification is made with a symbolic computation tool. The database presently contains information for 44 families of extremal graphs. For each of them, formulae giving the values for the 20 invariants in function of n have been obtained. This is usually an easy task using AGX 2. In a few cases however, *e.g.* for the index λ_1 for some families, no formula could be found.
In the experiments described in this paper, approaches (*i*) and (*iii*) are used. The approach (*iii*) has also been adapted to prove simple conjectures: the relevant families of extremal graphs for the invariants i_1 and i_2 are considered and if they have a non-empty intersection a proved and best possible bounding function is obtained. Moreover, this reasoning can be extended to consider the second best values as explained and illustrated in Section 4.

3 Experiments

We need a few definitions. Let $G = (V, E)$ denote a graph with vertex set V, $n = |V|$ vertices *i.e.*, of *order* n, edge set E and $m = |E|$ edges *i.e*, of *size* m. An edge e_k is a pair of vertices $\{v_i, v_j\}$, with which e_k is *incident*, and which are *adjacent*. The *adjacency matrix* $A = (a_{ij})$ is such that $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$ otherwise. The largest eigenvalue λ_1 of the matrix A is the *index* of G.
A *path* joining v_i and v_j is a sequence of edges such that v_i is the first vertex of the first edge, the second vertex of each edge is the first one of the next edge and so on, and the second vertex of the last edge is v_j. If $v_i = v_j$ the path becomes a *cycle*. The *length* of a path (cycle) is the number of its edges. The length of the shortest cycle of G is called its *girth* and noted g. The *distance* l_{ij} between vertices v_i and v_j is the length of a shortest path joining v_i and v_j. One of the invariants we will consider is the *average distance* between pairs of vertices, noted $\bar{l}$. If there is a path between any pair of vertices v_i and v_j of G, then G is *connected*. In this paper, we only consider connected graphs, moreover, to avoid border effects, we assume that the order of G is at

least 3. The largest distance between a vertex v_i and another vertex of G is v_i's *eccentricity*; the minimum eccentricity of a vertex of G is G's *radius* r and the maximum is G's *diameter* D. The *average eccentricity* is noted *ecc*. The sum of distances between a vertex v_i and all others is v_i's *transmission*. In order to better compare such values with the eccentricity, a normalization, *i.e.*, dividing by $n-1$, is appropriate: then the *normalized transmission* of v_i is the *average distance* to all other vertices of G. We call the minimum normalized transmission of G its *proximity*, noted π, and the maximum its *remoteness*, noted ρ. The *degree* d_i of a vertex v_i is the number of edges of G incident with v_i. We denote by Δ, $\overline{d}$ and δ respectively the *maximum, average* and *minimum degree* of G. The *Randić index* [47] of G is defined by

$$R = \sum_{i,j|\{v_iv_j\}\in E} \frac{1}{\sqrt{d_id_j}}; \tag{3}$$

where d_i denotes the degree of a vertex v_i. It is used extensively in mathematical chemistry. The *Laplacian matrix* L of G is defined by: $L_{ii} = d_i$ and $L_{ij} = -a_{ij}(i \neq j)$ where d_i is the degree of the vertex i and $A = (a_{ij})$ is the adjacency matrix of the graph. The second smallest eigenvalue of L, noted a, is the *algebraic connectivity* of G. The smallest number, ν, of vertices whose deletion disconnects a graph G or reduces it to a single vertex is G's (*node*) *connectivity*. The smallest number, κ, of vertices whose deletion disconnects a graph G is its *edge connectivity*. The *independence number* α of G is the cardinality of a largest set of pairwise non-adjacent vertices. The *clique number* of G is the maximum cardinality of a set of pairwise adjacent vertices. A vertex subset S of G is *dominant* if any vertex is in S or has a neighbor in S. The minimum cardinality of a dominant set is the *domination number* and is denoted by β. The *matching number* μ of G is the smallest number of pairwise disjoint edges.

A graph is *complete*, and noted K_n, if all pairs of vertices are adjacent; it is a *tree* if it is connected and has no cycles; it is a *star* if it is a tree and has a dominant vertex, *i.e.*, a vertex adjacent to all others; it is *bipartite* if it consists of two sets, of order p and q, of pairwise non-adjacent vertices, and edges joining vertices from one set to vertices of the other; it is *complete bipartite*, and noted $K_{p,q}$, if it contains all such edges. An edge with a vertex of degree 1 is a *pending* edge. A *cut vertex* is a vertex whose removal disconnects the G; a *cut edge* (or *bridge*) is an edge whose removal disconnects the G.

Inv.	**Name**	**Lower bound** $\underline{b}(n)$	**Extremal graphs for** $\underline{b}(n)$	**Upper bound** $\overline{b}(n)$	**Extremal graphs for** $\overline{b}(n)$
Δ	Maximum degree	2	P_n, C_n	$n-1$	G with a dominating vertex (K_n, S_n, $\ldots$)
δ	Minimum degree	1	G with a pending vertex (Tree, P_n, S_n, $\ldots$)	$n-1$	K_n

$\overline{d}$	Average degree	$2-\frac{2}{n}$	Tree (P_n, S_n, ...)	$n-1$	K_n
$\overline{l}$	Average distance	1	K_n	$\frac{n+1}{3}$	P_n
D	Diameter	1	K_n	$n-1$	P_n
r	Radius	1	G with a dominating vertex (K_n, S_n, ...)	$\lfloor \frac{n}{2} \rfloor$	P_n, C_n, ...
g	Girth	3	G with a triangle (K_n, ...)	n	C_n
ecc	Average eccentricity	1	K_n	$\frac{3n+1}{4} \cdot \frac{n-1}{n}$ if n is odd $\frac{3n-2}{4}$ if n is even	P_n
π	Proximity	1	G with a dominating vertex (K_n, S_n, ...)	$\frac{n+1}{4}$ if n is odd $\frac{n}{4}+\frac{n}{4n-4}$ if n is even	P_n and C_n
ρ	Remoteness	1	K_n	$\frac{n}{2}$	P_n
λ_1	Index	$2cos\frac{\pi}{n+1}$	P_n	$n-1$	K_n
R	Randić index	$\sqrt{n-1}$	S_n	$\frac{n}{2}$	G regular (K_n, C_n, ...)
a	Algebraic connectivity	$2-2cos\frac{\pi}{n}$	P_n	n	K_n
ν	Node connectivity	1	G with a cut vertex	$n-1$	K_n
κ	Edge connectivity	1	G with a cut edge	$n-1$	K_n
α	Independence number	1	K_n	$n-1$	S_n
β	Domination number	1	G with a dominating vertex (K_n, S_n, ...)	$\lfloor \frac{n}{2} \rfloor$	$K_{\lceil \frac{n}{2} \rceil} + \lfloor \frac{n}{2} \rfloor$ disjoint pending edges
ω	Clique number	2	C_n, P_n, Tree, ...	n	K_n
χ	Chromatic number	2	G bipartite, (Tree, P_n, ...)	n	K_n
μ	Matching number	1	S_n	$\lfloor \frac{n}{2} \rfloor$	K_n, P_n, C_n, ...

Table 1: Selected invariants together with lower and upper bounds for all connected graphs with at least 3 vertices.

The 20 selected invariants are listed in Table 1 together with their lower and upper bounds as functions of n and the corresponding extremal graphs. This was input for the system. Note that from the definitions, and known results [19, 25, 33]:

$$\delta \leq \overline{d} \leq \lambda_1 \leq \Delta; \;\; \pi \leq r \leq \alpha; \;\; r \leq D; \; \pi \leq \overline{l} \leq \alpha; \;\; \overline{l} \leq D; \;\; \overline{l} \leq \rho. \tag{4}$$

These relations were also considered as input, together with the further relations of [33] $\alpha \leq n - \delta$; $\alpha \leq n - r$; $R \leq \frac{n}{2}$; $r \leq D \leq 2r$ which are proved or folklore.
When a pair of invariants are combined together with an operation $\oplus$, AGX 2 first checks if there is a known and tight bound or if one can be derived from Table 1. If yes, this relation is given as output. Otherwise, presumably extremal graphs are sought. Then the numerical method is applied to find $\underline{b}(n)$ or $\overline{b}(n)$. If it succeeds, AGX 2 then checks if the relation follows from known equalities or inequalities. Otherwise, it examines whether extremal graphs correspond to a known family, for which formulae giving the value of the invariants as functions of n are known. If so, they are substituted, the resulting expression possibly simplified and given as output. If not, the structural result, or the presumably optimal graphs if none was found, are the output, to be studied unassisted or with the interactive component of AGX 2.

4 Results

There are 1520 cases. In each case graphs with 5 to 20 vertices were considered. Computing time on Intel Xeon with 2.66 GHz and 2 Gb RAM, varied from less than 1 second in the frequent case in which a bound could be obtained automatically, without using VNS, up to 75 seconds per graph in the most complex cases, weither results were obtained or not. Trying longer computing times did not give better results.
All results will be posted in a site under construction. They break down as follows.

4.1 Known results reproduced (37 cases)

AGX 2 reproduced, without making use of them, the 4 known relations $r \leq \alpha$; $\overline{l} \leq \alpha$; $\alpha \leq n - r$ and $\alpha \leq n - \delta$ of [33] which are proved and tight. The system also obtained further relations of the list (4) or which follow by transitivity, and which are also tight. (It is quite possible that some other relations among those found are known and described somewhere in the vast graph theory literature).

4.2 Complete results following from definition (32 cases)

When both invariants considered come from the same vector or matrix, say S, by taking its minimum ($m = minS$), average $\overline{s} = (\sum_{s \in S} s)/|S|)$ or maximum value ($M = maxS$), it is obvious that

$$m \leq \overline{s} \leq M$$

with equality if and only if the entries of S are equal. Immediate consequences of this double inequality are

$$M - \overline{s} \geq 0, \quad \overline{s} - m \geq 0, \quad M - m \geq 0, \quad \frac{M}{\overline{s}} \geq 1, \quad \frac{\overline{s}}{m} \geq 1 \quad \text{and} \quad \frac{M}{m} \geq 1.$$

Example 1 (Observations 1 and 2) **:** *For all connected graphs G with $n \geq 3$ vertices, radius r, diameter D and average distance $\overline{l}$,*

$$D - \overline{l} \geq 0 \quad \textit{and} \ \frac{D}{\overline{l}} \geq 1.$$

Moreover, the equality holds, in both cases, if and only if G is a complete graph.

The above inequalities follow from the fact that the diameter D is the maximum of all distances between pairs of vertices, and the average distance $\overline{l}$ is the average of all such distances.

4.3 Complete results proved from intersection of families of extremal graphs (776 cases)

Example 2 (Observations 3 to 6) **:** *For all connected graphs G with $n \geq 3$ vertices, Randić index R and radius r*

$$1 + \sqrt{n-1} \leq R + r \leq \tfrac{n}{2} + \left\lfloor \tfrac{n}{2} \right\rfloor, \tag{5}$$

and

$$\sqrt{n-1} \leq R \cdot r \leq \tfrac{n}{2} \cdot \left\lfloor \tfrac{n}{2} \right\rfloor, \tag{6}$$

Moreover, the equality holds for both lower bounds if and only if G is a star, and for both upper bounds if and only if G is a cycle.

Proof : From Table 1, the star is the only graph that minimizes the Randić index R and the radius r (also called the *centric index* [9] in chemical graph theory); the complete graph is the only graph that simultaneously minimizes α and maximizes R. The results follow. □

4.4 Complete results proved from recognizing extremal graphs and using second extremal value (33 cases)

Example 3 (Observation 7)**:** *For any connected graph G with $n \geq 4$ vertices, diameter D and average degree $\overline{d}$*

$$4 - \frac{4}{n} \leq D \cdot \overline{d} \tag{7}$$

Moreover, the bound is attained if and only if G is a star.

Proof : If $D = 1$, G is a complete graph, with $\overline{d} = n - 1$ and $D \cdot \overline{d} = n - 1$. If $D \geq 2$, as G is connected $\overline{d} \geq 2 - \frac{2}{n}$ and the lower bound follows by multiplication. Moreover $\overline{d} = 2 - \frac{2}{n}$ implies that G is a tree, and $D = 2$ that it is a star. □

4.5 Complete results proved or refuted by hand or in an assisted way or still open (419 cases: 349 proved, 54 open, 16 refuted)

Example 4 (Proposition 1)**:** *For any connected graph G with $n \geq 3$ vertices, average distance $\bar{l}$ and Randić index R*

$$R \cdot \bar{l} \leq \frac{n+1}{3} \cdot \frac{n-3+2\sqrt{2}}{2}. \tag{8}$$

Moreover, the bound is attained if and only G is a path.

Proof : If $m = n-1$, *i.e.,* G is a tree, it is known that both the Randić index and the average distance are maximum for the path [27, 51]. If $m \geq n$, $R \leq \frac{n}{2}$ (as for all graphs, [33]). Moreover, removing edges one at a time without disconnecting G or eliminating all cycles augments strictly $\bar{l}$. Thus G must have $m = n$ edges. Then, the maximum average distance of a graph G is attained for a triangle with an appended path of length $n-3$. It follows by easy computations that for $m \geq n$

$$\bar{l} \leq \frac{(n^3-7n+12)}{3n(n-1)} \leq \frac{n}{3},$$

and

$$R \cdot \bar{l} \leq \frac{n}{2} \cdot \frac{n}{3} < \frac{n+1}{3} \cdot \frac{n-3+2\sqrt{2}}{2}.$$

This completes the proof. □

Example 5 (Proposition 2)**:** *For any connected graph G with $n \geq 3$ vertices, remoteness ρ and maximum degree Δ*

$$\rho + \Delta \leq n + 1 - \frac{1}{n-1}. \tag{9}$$

Moreover, the bound is attained if and only if G has at least one dominant vertex and one pending edge.

The proof [1], which takes 2/3 of a page, is omitted here.

Example 6 (Theorem 1)**:** *For any connected graph G with $n \geq 3$ vertices, index λ_1 and average distance $\bar{l}$*

$$\lambda_1 + \bar{l} \leq n. \tag{10}$$

Moreover, the bound is attained if and only if G is a complete graph.

A proof, which is several pages long, as well as a shorter one for a stronger result are given in [5].

We next turn to cases in which AGX 2 only provides structural conjectures.

4.6 Structural conjectures followed by algebraic conjectures obtained by hand or in an assisted way (86 cases: 40 proved, 40 open, 6 refuted)

A first reason for not obtaining algebraic relations in an automated way is that extremal graphs may belong to 2 or more families.

Example 7 (Proposition 3)**:** *For any connected graph G with $n \geq 3$ vertices, Randić index R and index λ_1*

$$R - \lambda_1 \leq \begin{cases} \frac{n-3+2\sqrt{2}}{2} - 2cos\frac{\pi}{n+1} & \text{if } n \leq 9 \\ (n-4)/2 & \text{if } n \geq 10 \end{cases} \tag{11}$$

$$R/\lambda_1 \leq \begin{cases} (\frac{n-3+2\sqrt{2}}{2})/(2cos\frac{\pi}{n+1}) & \text{if } n \leq 26 \\ n/4 & \text{if } n \geq 27 \end{cases} \tag{12}$$

Moreover, in the case of the difference, equality holds if and only if G is a path for $n \leq 9$, and a cycle for $n \geq 10$; in the case of the ratio, equality holds if and only if G is a path if $n \leq 26$, and a cycle if $n \geq 27$.

Proof : Difference: If $m = n - 1$, *i.e.,* the graph is a tree, it is known that R is maximum and λ_1 is minimum for a path [25]. Then substituting values of R and λ_1 as functions of n gives the first relation of (11). If $m \geq n$, it is also known that R is maximum and λ_1 is minimum for a cycle. Then substituting values for R and λ_1, *i.e.,* $\frac{n}{2}$ and 2 gives the second relation of (11). Easy algebraic manipulations show when one bound is better than the other.
Ratio: The proof follows similar lines as for the difference; it is therefore omitted here. □
Another reason for difficulty in getting explicit algebraic relations is that some invariants such as the index rapidly imply complicated computations.

Example 8 (Theorem 2)**:** *For any connected graph G with $n \geq 3$ vertices, index λ_1 and minimum degree δ*

$$1 \leq \lambda_1/\delta \leq n - 2 + t, \tag{13}$$

and

$$0 \leq \lambda_1 - \delta \leq n - 3 + t, \tag{14}$$

where t satisfies $0 < t < 1$ and the equation $t^3 + (2n-3)t^2 + (n^2 - 3n + 1)t - 1 = 0$. The lower bound, in both cases, is attained if and only if G is a regular graph, and the upper bound, in both cases, is attained if and only if G is a graph which is a "short kite", i.e., a clique on $n - 1$ vertices with a pending edge.

The proof (see [5]) involves long algebraic manipulations and is omitted here.
Some relations are difficult to obtain in an automated way as well as to prove. A first reason may be the presence of floor or ceiling operators: $\lfloor x \rfloor$ denotes the floor of x, *i.e.*, the largest integer not larger than x and $\lceil x \rceil$ denotes the ceiling of x, *i.e.*, the smallest integer not smaller than x.

Example 9 (Conjecture 1)**:** *For any connected graph G with $n \geq 3$ vertices, Randić index R and independence number α*

$$R \cdot \alpha \leq \left\lceil \frac{3n-2}{4} \right\rceil \sqrt{\left\lceil \frac{3n-2}{4} \right\rceil \left\lfloor \frac{n+2}{4} \right\rfloor}. \tag{15}$$

Moreover, the bound is attained if and only if G is a complete bipartite graph K_{pq} with $p = \alpha = \lceil \frac{3n-2}{4} \rceil$ and $q = \lfloor \frac{n+2}{4} \rfloor$.

4.7 Structural conjectures only (82 cases: 5 proved, 77 open, 0 refuted)

Example 10 (Conjecture 2)**:** *Among the set of all connected graphs on $n \geq 3$ vertices with index λ_1 and average degree $\overline{d}$, some pineapples, i.e., a clique together with pending edges all incident with the same vertex from the clique and each with a vertex of degree one, maximize $\lambda_1 - \overline{d}$.*

This conjecture remains open and no formula for bounding $\lambda_1 - \overline{d}$ from above is known for such graphs [2]. Note that $\lambda_1 - \overline{d}$ was proposed as an irregularity index in [20]. It is compared with other irregularity indices in [36].

4.8 No results as extremal graphs are too irregular (55 cases)

5 Comparison of AGX 2 with other systems

In this section, we compare formulae obtained in our experiments with similar or simpler ones found by the systems GRAPH, GRAFFITI and HR, when available. Note that this comparison is limited as all systems cited can and do find formulae which do not fit in AGX Form 1.

5.1 GRAPH

The GRAPH system, which pioneered the man-machine type of research in graph theory, was developed by Cvetković and co-workers [23, 24] between 1980 and 1984. This system was extensively used to find conjectures and prove theorems in graph theory (usually the latter only being published), with an emphasis on algebraic graph theory. It comprises a bibliographic component (BIBLI), a theorem proving component (THEOR) and an algorithmic component (ALGOR). We focus on the last one.

ALGOR is directly connected to conjecture-making. The aim of this component is checking, disproving or making conjectures in graph theory. ALGOR solves a series of problems on particular graphs: setting and displaying values of the mentioned objects, creating common or random graphs, obtaining new graphs by performing graph-theoretic operations, relabeling graphs, determining integer or real invariants of a graph, checking properties of graphs and listing families of graph characteristics.

Using GRAPH, Cvetković and his collaborators got, among many others, the following results:

Example 11 (Theorem 3 [25])**:**
(i) If T is a tree of index $\lambda_1(T)$, then

$$2cos(\frac{\pi}{n+1}) \leq \lambda_1(T) \leq \sqrt{n-1}.$$

Equality holds if the graph is a path for the lower bound, and if and only if the graph is a star for the upper bound.
(ii) If U is a unicyclic graph of index $\lambda_1(U)$, then

$$2 \leq \lambda_1(U) \leq \lambda_1(S_n + e),$$

where $S_n + e$ is a star with an added edge. Equality holds if the graph is a cycle for the lower bound, and if and only if the graph is $S_n + e$ for the upper bound.

The bounds stated in Example 11 were tested using AGX 2, and reproduced in different ways. The lower bound in (i) is obtained automatically as a structural conjecture, and then, the algebraic expression is $\lambda_1(P_n)$, where P_n is a path on n vertices. The upper bound of (i) and the lower bound in (ii) are obtained automatically as conjectures (both structural and algebraic). The upper bound of (ii) is obtained as a structural conjecture by AGX and no algebraic expression could be obtained. Many results obtained with the help of GRAPH are discussed in the survey [24]. As, with a few exceptions, they do not fit into AGX Form 1, comparison with this system was not pursued further.

5.2 GRAFFITI

The GRAFFITI system is due to Fajtlowicz [26, 31, 32] and was developed since the mid-eighties, with from 1990 onward collaboration of DeLaVina, notably in the development of its *Dalmatian* version. This system generates a large number of *a priori* conjectures, under the form of algebraic relations between graph invariants, then selects among them, by eliminating false or uninteresting conjectures through testing them on a database of graphs, applying heuristics and building counter-examples. Conjectures which pass these correctness and interestingness tests are proposed, after further selection, to the mathematical community in the large electronic file *Written on the Wall* [33].
Eight conjectures of this file involve 2 invariants of the set of 20 given in Table 1, and possibly the order n of the graph.
In 4 cases, proved GRAFFITI conjectures were reproduced using the AutoGraphiX system, but under the AGX Form 1. They are the following :

GRAFFITI form :	$\alpha \leq n - \delta;\;\; \alpha \leq n - r;\;\; r \leq \alpha;\;\; \bar{l} \leq \alpha.$
AGX Form 1 :	$3 \leq \alpha + \delta \leq n;\;\; 2 \leq \alpha + r \leq n;\;\; r - \alpha \leq 0;\;\; \bar{l} - \alpha \leq 0.$

In addition to the difference in form, the AutoGraphiX conjectures give the structure of extremal graphs associated to the bounds, *e.g.* the lower bound on $\alpha + \delta$ is attained for path-complete

graphs [50] of diameter 2 or 3, and the upper bound on $\alpha + \delta$ is attained for a graph that is the complement of a Turan graph (a set of disjoint cliques of order as equal as possible). Note that, as pointed out by an anonymous referee, it is shown in [11] that $\alpha + \delta \leq n$ with equality if and only if the complement of G has a component consisting of a clique and all other components (if any) have maximum degree less than or equal to that of the degree of the clique.
In another case, the open GRAFFITI conjecture $a \leq n/\bar{l}$ was also reproduced.
In the 3 remaining cases, AGX 2 was able to improve upon GRAFFITI conjectures. One of the stronger results, next discussed could be proved and led in turn to a proof of the open GRAFFITI conjecture mentioned.

Example 12 (Proposition 4)**:** *For any connected graph G with $n \geq 2$ vertices, minimum degree δ and average distance $\bar{l}$.*

$$\delta \cdot \bar{l} \leq n - 1. \tag{16}$$

Moreover, the bound is attained if and only if G is complete.

Proof: According to Beezer *et al.* [10],

$$\bar{l} \leq \frac{(n+1)n(n-1) - 2m}{(\delta+1)n(n-1)} = \frac{n+1}{\delta+1} - \frac{2m}{n} \cdot \frac{1}{(\delta+1)(n-1)}.$$

If we substitute $\frac{2m}{n}$ by $\bar{d}$, multiply by δ, and use the fact that $\delta \leq \bar{d}$, we get

$$\bar{l} \cdot \delta \leq (n + 1 - \frac{\bar{d}}{n-1})\frac{\delta}{\delta+1} \leq (n + 1 - \frac{\delta}{n-1})\frac{\delta}{\delta+1}.$$

The last expression is maximum if and only if $\delta = n - 1$, *i.e.*, when the graph is complete. (This proof was obtained by the first author in April 2004; another proof was obtained independently by B. Smith [49] from the AGX 2 conjecture). □
Formula (16) improves upon the conjecture WOW 127 of GRAFFITI, $\delta \cdot \bar{l} \leq n$. It has several consequences: (i) conjecture WOW 62, $d \cdot \bar{l} \leq n$, where d is the common degree of the vertices of a regular graph, is immediately improved to $d \cdot \bar{l} \leq n - 1$, which is also sharp; ($ii$) recall that the *chromatic number* χ of a graph G is the smallest number of colors to be assigned to G's vertices such that no pair of adjacent vertices have the same color. Conjecture WOW 231, *if G is a regular connected graph,* $\chi \cdot \bar{l} \leq n$ is sharpened to *if G is a regular connected but not complete graph,* $\chi \cdot \bar{l} \leq n - 1$; ($iii$) recall that the Laplacian matrix of a graph G is defined by $L = D - A$ where D is a diagonal matrix with degrees of G's vertices on the main diagonal and A is the adjacency matrix of G. Let a denote the *algebraic connectivity* of G [35], which is equal to the second smallest eigenvalue of L. Then conjecture WOW 128, $a \cdot \bar{l} \leq n$ can be proved. Indeed, it is known (see *e.g.* [35]) that

$$a \leq \frac{n}{n-1}\delta \tag{17}$$

and the result follows by substituting for δ. Moreover, if G is not a complete graph $a \leq (n-1)/\bar{l}$ (WOW 128 was open since 1988 and studied by several researchers).

As another example, AGX 2 reproduced automatically the improvement, already obtained by AGX 1 [16], of WOW 3, $\bar{l} \leq R$ for all connected graph G, to

$$R - \bar{l} \geq \sqrt{n-1} - 2 + \frac{2}{n} \tag{18}$$

and the bound is tight for stars.

5.3 HR

The system *HR* (for *Hardy - Ramanujan*), due to S. Colton [21], is a program which forms concepts and makes conjectures in pure mathematics such as group, number and graph theory. It represents pure mathematics concepts as data-tables, and definitions for concepts can be generated when needed, using information about how they were constructed. It operates on the data-tables according to a set of 10 production rules to turn old concepts into new ones, and uses parameters to detail what to do. HR comprises a routine that estimates whether and how much a concept is interesting, then it generates new concepts using only the interesting old ones. During the concepts formation (*e.g.* equivalence between two concepts), some empirical evidence appear and then HR states them as conjectures. Colton [22] sent us a series of 259 algebraic relations conjectured by HR and tested on all graphs with up to 6 vertices. Of these, 6 were bounds on single invariants in terms of n, present in Table 1; 28 other conjectures involve 2 invariants of the set of 20 given in Table 1, as well as, possibly the order n of the graph; in 18 of these 28 cases AGX 2 reproduced the HR conjecture; in the remaining 10 cases, AGX 2 gave stronger conjectures than HR. It would be noted, however, that in 5 cases of these 10 the improvement is only due to a border effect, HR considering all graphs and AGX 2 all connected graphs with at least 3 vertices. In the 5 remaining cases, AGX 2 gave better results than HR.

Example 13 : *For all connected graphs G with $n \geq 2$ vertices, average degree $\overline{d}$ and minimum degree δ*

$$\overline{d} + 2 \leq n + \delta \qquad \textit{(HR)}$$

and

$$\overline{d} - \delta \leq n - 4 + \tfrac{4}{n} \qquad \textit{(AGX 2)}$$

moreover this last bound is tight if and only if G is a clique on $n-1$ vertices with a pending edge.

Proof: For any graph G of minimum degree δ and size m, we have

$$m \leq \delta + \frac{(n-1)(n-2)}{2}.$$

Then

$$\overline{d} - \delta = \frac{2m}{n} - \delta \leq \frac{2\delta}{n} + \frac{(n-1)(n-2)}{n} - \delta = \frac{2-n}{n}\delta + \frac{(n-1)(n-2)}{n}.$$

The last expression being maximum if and only if $\delta = 1$ and the corresponding extremal graph is composed of a pending vertex together with all possible edges between the $n-1$ other vertices. $\square$

Note that using a recent function of AGX 2, which proves algebraic relations from a database of known ones by substitution of variables, 205 of the 259 relations were shown to hold, 16 more were proved by hand, 37 refuted and one remains open.

6 Conclusions

A systematic comparison of graph invariants has been made using AGX 2. Results are summarized in Table 2. The following conclusions can be drawn from this table: (*i*) complete results are obtained in the vast majority of cases (85.33 %); among these a few known results were reproduced (2.43 %) and a large number were proved automatically (55.33 %); a substantial number were proved by hand (22.96 %); some remain open (3.55 %) and a few were refuted (1.05 %). (*ii*) Among remaining cases structural results were obtained again in a large majority of cases (11.05 %, of all cases, or 75.34 % of the remaining cases); a larger proportion of structure results than of complete results remain open (8.36 % of all cases, or 75.6 % of structural results). (*iii*) No results were obtained in some cases (3.62 %); they correspond to cases where AGX 2 could not find families of extremal graphs or, more frequently, where extremal graphs exhibit no regularity. (*iv*) Only a very small proportion of the conjectures turned out to be false (1.38 %).

Known results reproduced	37	(2.43 %)
Complete results following from definition	32	(2.11 %)
Complete results proved by intersection rule	776	(51.05 %)
Complete results proved by second value rule	33	(2.17 %)
Complete results proved by hand	349	(22.96 %)
Open complete results	54	(3.55 %)
Refuted complete results	16	(1.05 %)
Proved structural results and formulae by hand	40	(2.63 %)
Open structural results and formulae by hand	40	(2.63 %)
Refuted structural results and formulae by hand	6	(0.4 %)
Proved structural results only	5	(0.33 %)
Open structural results only	77	(5.07 %)
Refuted structural results only	0	(0.00 %)
No results	55	(3.62 %)
Total	1520	(100 %)

Table 2: Summary of results.

To conclude, it appears that AGX 2 clearly performs well in obtaining best possible relations of the AGX Form 1 and corresponding extremal graphs. Moreover, easy results are proved automatically and others require short or sometimes somewhat longer proofs (mentioned but not given in this paper) or remain open.

In future work we plan to (*i*) present in detail in several papers currently in preparation the results obtained for each of the main invariants together with their proofs (when we found some); (*ii*) improve AGX 2's discovery abilities in various ways, based upon the insights gained by the experiments described; (*iii*) enrich that system by adding routines for computing many more graph invariants and performing operations on graphs; (*iv*) obtain many more conjectures and make them available at large; (*v*) consider different forms of algebraic conjectures then AGX Form 1, *e.g.* an AGX Form 2 where the bounding functions would depend on both the order n and the size m of the graphs under study; (*vi*) extend AGX 2 to tackle conjectures with a different logical structure than those of AGX Form 1 and Form 2, *e.g.* sufficient conditions for graphs to belong to a given family [39].

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