# Computers and Discovery in Algebraic Graph Theory

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#### Abstract

We survey computers systems which help to obtain and sometimes provide automatically conjectures and refutations in algebraic graph theory.

#### Résumé

On passe en revue les systèmes informatiques qui aident à obtenir et parfois donnent automatiquement des conjectures et réfutations en théorie algébrique des graphes.

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#### 1 Introduction

As already stressed by Archimedes [5] discovery and proof are different activities, which require different methods. One must first find what is to be proved, i.e., a conjecture, by any procedure, possibly aided by a physical model, then prove it or refute it by logical means. Both tasks can be aided by computers in various fields of mathematics. Fully automated proofs in graph theory are still limited to simple properties [50][51][52][56][64][65][66]. In contrast, partly automated proofs, which use both human reasoning and specialized computer programs, have met with much success since the proof of the 4-color theorem [2][3][4][116] (and despite the controversy on the reliability of such proofs, see e.g. [11]). To illustrate, the fifth update of a "dynamic survey" on "Small Ramsey Numbers" [112] reviews results which were obtained with the aid of the computer in 71 papers among the 274 which are cited. Recourse to the computer to complete a difficult proof is thus widespread.

In this paper, we focus on computer aids to discovery, i.e., finding conjectures and refutations, in graph theory. Examples come from algebraic graph theory.

Quite a few systems have been developed in the last 25 years. They are based on different principles, which can be regrouped as follows :

- (i) enumeration;
- (ii) interactive computing;
- (iii) invariant manipulation;
- (iv) generation and selection;
- (v) heuristic optimization.

Representative systems of each family are discussed in the next five sections and brief conclusions are given in the last one.

### 2 Enumeration

Enumeration refers to two distincts operations in mathematics performed, when examining a set of objects or structures. On the one hand, one can find how many there are, i.e. *count* them. Methods to do so are well developed in combinatorial mathematics and graph theory (see e.g. the books [91] [107]). On the other hand, one may consider each of them in turn, i.e., *list* them (this is sometimes referred to as constructure enumeration). Computer aids to discovery which use enumeration mostly address the second type of problem. To illustrate, recall that the *Folkman number*  $F_e(3,3,5)$  is defined as the smallest positive integer n such that there exists a  $K_5$ -free graph on nvertices for which every 2-coloring of its edges contains a monochromatic triangle. In [106] this number was proved to be equal to 15 by a careful enumeration, exploiting characteristics of graphs with the desired property.

Basic problems of enumeration are to avoid duplication and to efficiently exploit properties of the class of graph under study to curtail the search. Often graphs are generated by adding one vertex at a time, and some adjacent edges. To avoid duplication, graphs are encoded and a unique *father* is assigned to any *son*. This principle of *orderly generation* was proposed in [73] [74] [114] [115]. Variants and extensions, including the *canonical path method* are discussed in [101][102]. Moreover, symmetry can be exploited both to avoid duplication and to accelerate the search. A recent survey of



Figure 1: A new family of bipartite integral graphs [7]

isomorphism rejection methods is [25]. Several systems do this, e.g. Nauty [101][102]. This system and others such as CoCo [75] [76] are used in the package GAP (Groups, Algorithms and Programming) [82]. When applied to problems on groups and graphs, the program GRAPE, which is a part of GAP led to several results [42] [46] [44] [43] [45] [108] [123] [124], e.g., the discovery of a new infinite family of 5-arcs transitive cubic graphs.

Some systems for enumerating graphs are specialized, e.g., MOLGEN [83] which is designed for molecular graphs, *Fullgen* for fullerenes [26] and *minibaum* for cubic graphs [24]. *CaGe* [27] generates graphs of different types often related to intersting chemical molecules.

Enumeration of families of graphs defined by given properties often leads to conjectures about them or refutations of such conjectures.

Let G = (V, E) denote a graph with n = |V| vertices (i.e., of order n) and m = |E|edges (i.e., of size m). Its adjacency matrix  $A = (a_{ij})$  is such that  $a_{ij} = 1$  if vertices  $v_i$  and  $v_j$  are adjacent and  $a_{ij} = 0$  otherwise. The polynomial  $P(\lambda) = det(\lambda I - A)$ is called *characteristic polynomial* of G. The spectrum of G is the set of solutions to  $P(\lambda) = 0$ , called eigenvalues, and noted  $S_p = (\lambda_1, \lambda_2, \ldots, \lambda_n)$  with  $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ . The first eigenvalue  $\lambda_1$  is called the index or spectral radius.

In [53] spectra of all graphs with up to 9 vertices are given. This lists refutes 5 conjectures of *Graffiti* ([67][69], see Section 5).

A graph is called *integral* if all its eigenvalues are integer. Such graphs are rare. In [6][7] it is shown that there are only 263 non-isomorphic connected integral graphs with up to 11 vertices. These graphs could be determined by enumeration of connected graphs using *Nauty* [101][102] and computation of their spectra. Such a lengthy process required a supercomputer. Larger integral graphs, but possibly not all of them for given n, could be obtained with an evolutionary algorithm, using as fitness function the sum of distances from eigenvalues to their closest integer (and variants thereof) [8].

A bipartite graph  $K_{pq}$  is composed of two independent sets, with p and q vertices respectively, and some edges joining pairs of vertices one in each set. It is *complete* if it contains such edges for all pairs. Among other results, examination of the 263 integral graphs suggested two new infinite families of integral graphs [7]. The first one is obtained from the complete bipartite graphs  $K_{p,p+2}$  for p = 1, 2, ... by appending an edge to each vertex of the smallest independent set (see Figure 1).

A split graph  $SP_{pq}$  is composed of a clique on p vertices, an independent set on q vertices and some edges joining pairs of vertices one in each of those sets. It is complete if it contains edges for all such pairs. It was observed in [88] [109] that complete split graphs are sometimes but not always integral (see Figure 2). Then, generation of all



Figure 2: Small integral complete split graph  $SP_{2,3}$ 

complete split graphs with  $n = p + q \leq 500$  and  $p \leq 50$ , and computation of their spectrum with the  $Matlab^{TM}$  [100] programming language, led to several conjectures, e.g.

Conjecture 1 All complete split graphs with

$$q = \left\lceil \frac{i}{2} \right\rceil + (p-1) \left\lfloor \frac{i}{2} \right\rfloor \left\lfloor \frac{i+2}{2} \right\rfloor$$

where i is a positive integer, are integral. Moreover if p is a power of a prime there are no other integral complete split graphs.

This conjecture is proved in [88].

# **3** Interactive computing

Numerous conjectures of graph theory are obtained by drawing small graphs on paper or blackboard, making hand or pocket calculator computations of invariants under study, reasoning upon their values, then modifying these graphs and computing the consequences. Such a process can be aided by the computer, exploiting its abilities to make very quick computations and represent graphs in a clear way. A pioneering system in this respect is *Graph* [54] [55] [57] developed during the period 1980 – 1984 in Belgrade. This system comprises three main components : *Algor* which implements graph algorithms for computing a series of invariants, as well as *Biblio* and *Theor* a bibliographic and a theorem-proving component respectively. These last two will not be discussed here.

Graph also displays the graph currently under study and allows interactive modifications on screen : addition or deletion of edges and / or vertices (this, of course allows any transformation). While Graph does not provide conjectures or proofs in an entirely automated way, it has proved to be very successful in suggesting conjectures through analysis of examples, and also in helping to get proofs by checking particular cases. The survey papers [49] [57] mention 55 papers by 16 mathematicians with results obtained up to 1992 with the help of Graph. Many further papers mentioning use of Graph have since appeared.

We next give a few examples of results obtained with aid of this system. Further theorems of algebraic graph theory obtained in this way are listed in Table 1. There,  $P_n$  denotes the path on *n* vertices,  $P_n^2$  its square, i.e., the graph obtained by joining by an edge pairs of vertices of  $P_n$  at distance 2, and  $\bigtriangledown$  the join of two graphs where all vertices of one are joined by an edge to all those of the other.

**Example 1** Unicyclic graphs with extremal index are characterized in [120] :

 Table 1: Some theorems obtained with the help of the Graph system

 Formula
 Ref.

If G is a tree (with  $n \ge 3$ ), then [99]  $\lambda_1(P_n) \le \lambda_1(G) \le \lambda_1(K_{1,n})$ If G is a maximal outerplanar graph (with  $n \ge 4$ ), then [117]  $\lambda_1(P_n^2) \le \lambda_1(G) \le \lambda_1(K_1 \bigtriangledown P_{n-1})$ If G is a connected graph and if G' is obtained from G by [121] splitting a vertex, then  $\lambda_1(G') \le \lambda_1(G)$ 

**Theorem 2** ([120]) Let G denote a unicyclic graph; then

$$\lambda_1(C_n) \le \lambda_1(G) \le \lambda_1(K_{1n} + e)$$

with equality if and only if G is the n-cycle  $C_n$  or the star with one additional edge  $K_{1n} + e$ .

**Example 2** Combining graph theoretical results and computer search with *Graph*, all connected, non-regular, non-bipartite integral graphs with maximum degree four were determined in [110][111]. This method was used also to find connected non-regular bipartite integral graphs with  $\Delta \leq 4$  [9] [10] as well as one class of connected 4-regular integral graphs [126]. Note that the search was not carried out as a brute-force one but as a man-machine interaction, many parts of the search space being discarded for graph theoretical reasons or by computational results.

**Theorem 3 ([110][111])** There are exactly 13 integral graphs which are connected non-bipartite and non-regular with maximum degree 4.

These graphs are represented on Figure 3.

In the last decade both libraries of graph algorithms and systems for graphs visualisation and/or editing have proliferated. We mention a few. *GraphBase* [94], *Leda* [103] and *Vega* [127] comprise efficient implementations of many graph algorithms. *GraphEd* [92] and its successor *Graphlet* [93], *VCG* [118], *CABRI-Graph* [37], *Link* [15] [16] [17] [18], *GGCL* (Generic Graph Component Library) [96] and other systems possess in addition an editor. *EDGE* [105], *Da Vinci* [81], *Grappa* [12] and other systems focus on graph vizualisation and editing. Note that graph drawing is a well developed research area, see, e.g., the surveys [60] [62] and the book [61].

Recent systems are often the outcome of the merge of several previous ones. This is for instance the case of Link which build upon the experience of the authors of



Figure 3: The 13 integral graphs of Theorem 3 [110][111]

Combinatorica [122], NETPAD [104], SetPlayer [14] and GraphLab [119]. The Link system led to a conjecture, still open, which if true would reveal the first known infinite set of infinite antichains of tournaments [95].

## 4 Invariant manipulation

Graph theory contains a large number of relations between graph invariants. A few of them are equalities, the other inequalities, often nonlinear in one or more parameters. They may involve conditions, which are themselves relations or properties defining classes of graphs, e.g. planar, bipartite, tree, etc. Logical variables associated with these classes may also be considered as invariants. Generalized relations are then obtained and are of the forms:

- (i) "If relation R<sub>1</sub> holds then relation R<sub>2</sub> holds"
  e.g. "If β<sub>0</sub> = 2 and χ ≥ 4 then n ≥ 11" [41] where β<sub>0</sub> denotes the *independence* number, i.e., the maximum number of pairwise non-adjacent vertices and χ the chromatic number of G, i.e., the minimum number of colors needed to assign a color to each vertex such that no pair of adjacent vertices have the same color.
- (ii) "If condition c holds then relation R holds" e.g. "If G is planar then  $a \leq 3$ " [38] where a denotes the arboricity of G.
- (iii) "If condition  $c_1$  holds then condition  $c_2$  holds" e.g. "If G is a tree then it is bipartite" (obvious).
- (iv) "If relation R holds then condition c holds" e.g. "If  $n \ge 6\delta$  and  $m > \frac{1}{2}(n-\delta)(n-\delta-1) + \delta^2$  then G is hamiltonian" [28] where  $\delta$  denotes the minimum degree of G and a hamiltonian graph contains a path going ones and only ones through every vertex.

In order to build the graph invariant manipulator system *Ingrid*, 458 relations between graph invariants have been gathered in [21][22]. They involve 37 graph invariants, 27 of which are integer-valued, 1 real-valued and 9 boolean. A representative subset of these relations, involving  $\lambda_1$ , is given in Table 2. Here  $\chi_1$  denotes the *edge chromatic number* or smallest number of colors needed to color edges so that no two incident edges have the same color; g denotes the *girth* or length of the smallest cycle of the graph considered.

Ingrid [20][23] was designed to assist researchers in obtaining precise information, in the form of intervals on invariant values, for incompletely specified graphs or classes of graphs. To this effect, some parameters are given specified values or intervals containing their values. Then rules deduced from the relations are applied to tighten intervals for all invariants. This is done in a systematic way, until stability is attained. A tracing function allows listing those relations which have led to the lower or upper bound of the final interval for an invariant.

Moreover, conjectures may be temporarily considered as theorems (proved relations) added to the system and the consequences tested. If the interval of feasible values for some invariant becomes empty, a contradiction has been found and the conjecture refuted.

Ingrid can contribute to graph theory in several ways :

Formula	Ref.	Formula	Ref.
$\lambda_1 \ge \frac{2m}{n}$	[13]	$\lambda_1 \le \sqrt{\frac{2m\alpha_0}{(\alpha_0+1)}}$	[21]
$\lambda_1 \leq \Delta$	[13]	$\chi \ge \frac{n}{n-\lambda_1}$	[48]
$a \le 1 + \lfloor \frac{\lambda_1}{2} \rfloor$	[97]	$\beta_0 \geq \frac{n}{n-\lambda_1} - \frac{1}{3}$	[63]
$\chi \ge \frac{2m}{(2m-\lambda_1^2)}$	[63]	if $\lambda_1 \leq \frac{\Delta}{2}$ then $\chi_1 = \Delta$	[80]
if $\lambda_1 \ge \sqrt{m}$ then $g = 3$	[53]	$\lambda_1 \geq \sqrt{\Delta}$	[98]
$\chi \le \lambda_1 + 1$	[13]	if $G$ is connected, then	
$\lambda_1 \geq \delta$	[13]	$\lambda_1 \ge 2\cos[\pi/(n+1)]$	[13]

Table 2: Some relations involving  $\lambda_1$  in the *Ingrid* system

# (i) Detecting existence of relations between invariants and sets of relations leading to them.

Consider a pair of invariants for which a relation is sought; vary one of them and check if the feasible interval of the other given by *Ingrid* varies also. If it is the case, a relation exists. To find it, consider which relations have been used, with the tracing function. Then derive the relation by algebraic manipulation. This last step is done by hand, but could be automated, for instance with *Mathematica*<sup>TM</sup> [128].

**Example 3** In [23] a relation is sought between the spectral radius  $\lambda_1$  and the vertex clique cover number  $\theta_0$ , i.e., the smallest number of cliques which cover all vertices. While both parameters had been much studied it did not appear that any relation between then was yet published. Keeping the order n fixed and varying  $\lambda_1$ , Ingrid detected a change in the upper bound of the interval for  $\theta_0$ . This was due to the use of the four relation

$$\Delta \le \lambda_1^2,$$
  

$$\beta_1 \ge \frac{n}{(\Delta+1)},$$
  

$$\theta_0 \le \alpha_1,$$

 $\operatorname{and}$ 

$$\alpha_1 \le n - \beta_1$$

where  $\Delta$ ,  $\alpha_1$  and  $\beta_1$  denote maximum degree, edge covering number (minimum number of edges needed to cover the vertices) and matching number (maximum

number of independent edges) respectively. It is then easy to derive the theorem

$$heta_0 \le n \left[ rac{\lambda_1^2}{(1+\lambda_1^2)} 
ight]$$

which is useful for small  $\lambda_1$ .

(ii) Refuting conjectures

**Example 4** It was asked in [47] whether there exists planar triangle-free graphs with exactly  $3\beta_0$  vertices. Conjecturing this was the case with the temporary theorem feature of *Ingrid*, as explained above, led to a negative answer.

(iii) Exploring dominance between relations

An inequality between graph invariants may be implied by one or several other inequalities. When it is the case, there is no need to add it to the system. To check this, the bound it gives can be compared with that given by *Ingrid* for various feasible values of the invariants involved.

Example 5 The bound

$$\lambda_1 \le -1 + \sqrt{1 + 8m}$$

was proposed in [125]. Varying m in *Ingrid* and observing the upper bound on  $\lambda_1$  and the relations used, it was found that the pair of relations

$$\chi \le \left\lfloor 1 + \frac{\sqrt{1+8m}}{2} \right\rfloor$$

and

$$\lambda_1 \le \sqrt{2m(\chi - 1)/\chi}$$

provided bounds which were usually better and never worse. This could then be proved analytically.

The question of which relations are undominated is considered in [90]. An inequality  $i_1 \geq (\leq) f(i_2, i_3, \ldots, i_n)$  between an invariant  $i_1$  and one or several others  $i_2, \ldots, i_n$  is sharp if for all values of the independent invariants compatible with the existence of a graph, there is a graph for which equality holds. A complete set of sharp inequalities between invariants  $i_1, i_2, \ldots, i_n$  is composed of 2n sharp lower and upper bounds for each invariant  $i_j$  in function of the others. Such a complete set for the order, size and independence number of graphs has been gathered and completed by the proof of a remaining case in [90].

Ingrid can also be used to help to solve practical problems in network design and for pedagogical purposes [23]. Discovery-based pedagogy in graph theory is also discussed in [37], [39] and [58].

#### **5** Generation and selection

The *Graffiti* system [67][68][70][71][72] is designed for automated generation of conjectures in graph theory (as well as in geometry, number theory and mathematical chemistry). It contains a database of relations and a database of examples, which are graphs which refuted some conjecture. *Grafitti* proceeds in two steps :

(i) Graph invariants  $i_1, i_2, \ldots i_p$  are selected and a large number of a priori relations between them are generated. They have simple forms, e.g. :

 $i_k \leq i_l$  or  $i_k \leq i_l + i_m$  or  $i_k + i_l \leq i_m + i_n$ ;

one invariant may also be replaced by a constant, usually 1; sometimes ratios or products of invariants are also considered. In fact, as an algebraic expression involving one or several graph invariants is itself a graph invariant, any such relation can be used.

Classes of graphs to be considered, e.g. general, triangle-free, bipartite, tree and so on are also specified.

 (ii) Selection is performed among relations (or conjectures) obtained in (i). They may be discarded or provisionally set aside.

The former happens

- (a) when a new relation does not appear to be informative. To this effect it is tested whether it provides a sharper value for some invariant than all other relations in the database on at least one of the stored examples, or
- (b) when a new relation is shown to be false for at least one of those graphs.

The latter happens

- (c) when a new relation is implied by an existing conjecture, or
- (d) when a new relation for a given class of graphs (e.g. trees) is not refuted by any example of a larger class (e.g. bipartite graphs), or
- (e) when invariants in a relation are too close one to another (i.e.  $i_k \leq i_l = i_k + 1$ );

note that the test for informativeness removes most but not all such relations.

To speed up the procedure, both databases are kept of moderate size. When a counter-example is found it is added to the database, the refuted relations removed and possibly others, which become informative, added. When a new relation is added, those which are no more informative are set aside.

False conjectures play an important role as the systematic addition of graphs refuting them to the database leads to increasingly strong conjectures. The aim is to find this strongest conjecture for which no counter-example is known. Selected conjectures are proposed to the mathematical community in the large *Written on the Wall* [67] file. Their status, i.e., proved, refuted or open is specified and regularly updated. Indications on partial proofs and generalizations of the conjectures are also given, with references.

Initially, conjectures were examined before inclusion in *Written on the Wall* and sometimes proved or refuted; more recently their selection is enterely automated.

Graffiti has attracted the attention of more than 80 graph theorists and has led to publication of several dozen papers [59], some well-known ones being [40] [77] [78] [79]. Initially, refutations was easy; in [19] 200 conjectures of *Graffiti* were tested on all graphs with up to 10 vertices and over 40 of them were refuted. The remaining early open conjectures seem to be more likely to hold and some of them appear to be hard to prove. Relations of *Graffiti* in algebraic graph theory were studied in depth in [79].

Num.	Formula	Status
WOW 19	$-\lambda_n \leq \chi$	Proved in [79]
WOW 43	If G is regular, $-\lambda_n \leq \beta_1$	Proved in [79]
WOW 44	If G is regular, $\lambda_2 \leq \beta_0$	Refuted by N. Alon
WOW 45	If G is regular, $\lambda_2 \leq \beta_1$	Proved by N. Alon
WOW 116	If G is triangle-free, $\lambda_1 \leq Ra$	Proved in [79]
WOW 195	$\lambda_n \leq \max(E^*)$	Open

m 11 a d 

We next give a few examples. Further relations and their status are presented in Table 3. There  $E^*$  denotes the vector whose  $i^{th}$  component is the number of vertices at even distance from the  $i^{th}$  vertex and Ra is the Randic [113] or connectivity index of a graph G = (V, E) defined as

$$Ra(G) = \sum_{(i,j)\in E} \frac{1}{\sqrt{d_i d_j}}$$

where  $d_i$  is the degree of vertex *i*.

Example 6 [Conjecture WOW 747, open] Let b be the order of the largest bipartite subgraph of a connected graph G, then the average distance between distinct vertices of G is not more than  $\frac{b}{2}$ .

Fajtlowicz observes that if true this conjecture would generalize the previous Conjecture WOW 2, i.e., that the average distance is not more that the independence number, which was proved in [40].

**Example 7** [Conjecture WOW 776, refuted] Let p be the sum of positive eigenvalues of G If G is cubic then the independence number of G is greater than or equal to  $-1 + \frac{p}{2}$ .

An 18-vertex counter-example was found in [109] using the AGX system (see Section 6). For that graph  $\beta_0 = 6$  and  $-1 + \frac{p}{2} > 6.04$ 

Example 8 [Conjecture WOW 256, proved] Let the dual degree of a vertex be the mean of the degrees of its neighborhoods. Then the maximum eigenvalue of the adjacency matrix of a graph G is not more than its maximum dual degree.

The same short and elegant proof for this result was found independently by a researcher in the U.S. and a group of three researchers in France, see [67], page 78. The result generalizes the well known property that the largest eigenvalue of G is not more than its maximum degree. The french group noticed that equality holds if and only if every vertex has the same dual degree.

### 6 Heuristic Optimization

Conjectures in graph theory can be viewed as combinatorial optimization problems on an infinite family of graphs (of which only those moderate order will be explored). Indeed, given a relation  $i_k \leq i_l$ , one can minimize over all graphs  $i_l - i_k$ , parameterizing for instance on the graph order. As soon as a graph such that  $i_l - i_k < 0$  is found the conjecture is refuted. Conversely if extremal or near-extremal values of an invariant (which may be an expression involving several other ones) are found for all small values of parameters such as order and size, this may lead, automatically or with the aid of the computer, to the discovery of new conjectures.

This is the approach on which the AutoGraphiX (AGX) system [1] [29] [30] [31] [32] [33] [34] [35] [36] [87] is based. AGX addresses the following problems :

- (a) find a graph satisfying given constraints;
- (b) find optimal or near-optimal values for an invariant subject to constraints;
- (c) refute a conjecture;
- (d) find (or suggest) a new conjecture (or sharpen an existing one);
- (e) suggest a proof strategy.

AGX uses extensively the Variable Neighborhood Search (VNS) metaheuristic (or framework for building heuristic) [89]. This metaheuristic exploits the relatively unexplored idea of systematic change of neighborhood within a local search. VNS starts with a given randomly generated initial solution (or graph)  $x_0$  then applies a descent routine (when minimizing) until a local optimum x is reached. Then a set of nested neighborhoods centered around x are considered and a point x' is randomly generated from the first neighborhood. A descent is performed from x', leading to a local optimum x''. If x'' = x or if the value of x'' is not better than that of x, the solution x'' is ignored and another solution x' is generated from the next neighborhood. Otherwise, as a better local optimum x'' than x has been found, the search is recentered there. When the last neighborhood has been considered one begins again with the first one until a stopping condition is met.

The descent routine may itself use several neighborhoods (of types of moves). AGX uses ten simple graph transformations for that purpose : *addition* of an edge, *removal* of an edge, *rotation* of an edge (i.e., change of one of its endpoints), *move* of an edge (i.e., deletion followed by addition, but not in the same position), and similar more complex changes.

Nested neighborhoods of a graph are defined by the Hamming distance between edge-sets : the first one consists of all graphs obtained by deletion or addition of a single edge, then two, and so on.

AGX has led, partly in conjunction with a program for enumerating cubic graphs [25] to refutation of 9 conjectures of *Graffiti* [36] [109] and to the discovery of over 50 new conjectures, 15 of which have been proved.

We next give a few examples of those results. Others are listed in Table 4. We recall a few definitions used there. A comet  $C_{p,t}$  is obtained from a star  $K_{p-1,1}(p \ge 4)$  by appending a path with t edges to a pending vertex. A double comet  $D_{p,t,q}$  is obtained from two stars on p and q vertices by joining a pending vertex of each of them with a path of t + 1 edges (see Figure 4). The radius r of graph G is the minimum over all

Table 4: Some results obtained with AGX

Num.	Num. Conjecture		Ref.
Co. AGX 13	If G is a graph with n vertices, $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ edges and	Open	[29]
	minimum energy, then		
	(i) if they are positive integer $a$ and $b$ such that $a \times b =$		
	m and $a+b \leq n$ , G is a complete bipartite graph $K_{a,b}$ possibly with additional isolated vertices		
	(ii) otherwise G is a complete bipartite graph $K_{a',b'}$		
	with $a' \times b' \leq m$ and $a' + b' \leq n$ , modified by addition		
	of $m - a' \times b'$ edges joining a vertex on the smallest		
	side on $K_{a',b'}$ to others vertices on that side, possibly		
Th ACY 19	with additional isolated vertices Let $\mathcal{T}_{-}$ denotes the family of trees with a black and	Droud	[20]
III. AGA 12	Let $\mathcal{J}_{a,b}$ denotes the family of frees with a black and b white vertices $a > b$ . Then for a fixed number of	rroveu	[30]
	vertices n and $T \in \mathcal{T}_{+}$ the minimal value of $\lambda_1$ of T		
	increases monotonously with $a - b$		
Th. AGX 13	For $a = b + 2$ and $n > 6$ , the trees $T^* \in \mathcal{T}_{a,b}$ with	Proved	[30]
	minimum index $\lambda_1$ are comets $C_{4,n-4}$ . Moreover		
	$\lim_{n\to\infty}\lambda_1(T^*)=2$		
	For $a = b + 3$ and $n \ge 7$ , the trees $T^* \in \mathcal{T}_{a,b}$ with minimum index $\lambda_1$ are double comets $D_{3,n-6,3}$ and $\lambda_1(T^*) = 2$ .		
Co. AGX 4	Let G be a graph with $n \ge 3$ vertices, then	Open	[34]
	$r + Ra - mode(d) \ge \sqrt{n-1} - 1$		
	(Reinforcement of <b>Conjecture WOW 7</b> )		



Figure 4: Color-constrained trees with minimum index : comets and double comets

vertices of the maximum distance from that vertex to any other.

Observe that they are of two types:

- (a) relations between graph invariants and
- (b) structure of extremal graphs.

**Example 9** The *energy* of a graph [84] [85] is defined as

$$E = \sum_{i=1}^{n} |\lambda_i|.$$

A study of graphs with extremal energy [29], parameterizing on n and m led, among others, to the conjectures

$$E \ge 2\sqrt{m}$$
 and  $E \ge \frac{4m}{n}$ .

Both of them have been easily proved.

**Example 10** In the same study, unicyclic graphs with maximum energy were investigated. This led to the following structural result.

**Conjecture AGX 16** Among unicyclic graphs with n vertices the cycle  $C_n$  has maximum energy if  $n \leq 7$  or n = 9, 10, 11, 13 and 15; otherwise the unicyclic graph with maximum energy is  $C_6 + P_{n-6}$  i.e.,  $C_6$  with an appended path with n - 6 edges.

Partial results towards the proof of this conjecture were recently obtained : it is shown in [86] that among bipartite unicyclic graphs those with maximum energy are either  $C_n$  or  $C_6 + P_{n-6}$ .

The results of these two examples were obtained interactively. However there are several ways to use AGX in an entirely automated way [34]. Indeed conjectures can be found by

- (i) a numerical procedure which exploits the mathematics of principal components analysis in order to find ressemblances instead of differences between extremal graphs. This leads, in polynomial time, to a basis of affine relations between graph invariants;
- (ii) a geometric procedure, i.e., finding the convex hull of the set of extremal graphs viewed as points in invariant space, facets of this convex hull give linear relations, i.e., lower and upper bounds on the invariants associated with each of the axes;
- (iii) an algebraic procedure, i.e., recognizing the class of extremal graphs found, and if it is a well-defined one for which formulae relating graph invariants are known, eliminating variables to get simple relations between the invariants under study.

**Example 11** In [30] color-constrained trees (i.e., trees with given numbers of black or white vertices) with minimum index are investigated. A further study of the extremal graphs found was performed in [34][35]. To this effect 15 graph invariants were computed and the numerical method applied. In addition to some trivial relations it led to the following result.

Conjecture AGX 9 In all color-constrained trees with minimum index

$$\beta_0 = \frac{1}{2} \left( m + n_1 + D - 2r \right)$$

where  $\beta_0$  denotes the independence number, m the size,  $n_1$  the number of pendent vertices, D the diameter and r the radius.

It is unlikely that a relation with as many invariants could have been obtained without a computer.

This conjecture is open; it does not hold for all trees. However it could be shown [34] that the right-hand side is an upper bound on the independence number of trees. So **Conjecture AGX 9** implies that color-constrained trees with maximum index have maximum independence number.

**Example 12** Using the geometric approach [34] to study chemical graphs (i.e., graphs with a maximum degree of 4) led to find :

Theorem AGX 5 In all chemical graphs

$$Ra \ge \frac{1}{4} \left( n_1 + m \right).$$

This was proved using linear programming arguments.

**Example 13** Conjecture 8 of Graffiti is that in a graph G

 $\bar{l} + Ra - \text{mode}(d) \ge 0$ 

where  $\overline{l}$  denote the average distance between of distinct vertices and d the vector of degrees of G. Using the algebraic approach led to the following strengthening of that result :

Conjecture AGX 5 In a graph G

$$\bar{l} + Ra - \text{mode}(d) \ge \frac{2(n-1)}{n} + \sqrt{n-1} - 2 \text{ if } n \ge 3.$$

#### 7 Concluding remarks

Several discovery systems in graph theory have been very succesful in helping mathematicians to formulate and explore conjectures, or to suggest interesting conjectures in an entirely automated way. Moreover, new systems sometimes based on new principles are being developed. The underlying paradigms, i.e., enumeration, interactive computing, formula manipulation, generation and selection, heuristic optimization, are varied. They appear to be largely complementary. So one may expect much activity and the advent of more comprehensive systems in the near future.

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