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What Forms Do Interesting Conjectures Have in Graph Theory ?

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Abstract

Conjectures in graph theory have multiple forms and involve graph invariants, graph classes, subgraphs, minors and other concepts in premisses and/or conclusions. Various abstract criteria have been proposed in order to find interesting ones with computer-aided or automated systems for conjecture-making. Beginning with the observation that famous theorems (and others) have first been conjectures, if only in the minds of those who obtained them, we review forms that they take. We also give examples of conjectures of such forms obtained with the help of, or by, computers when it is the case. It appears that many forms are unexplored and so computer-assisted and automated conjecture-making in graph theory, despite many successes, is pretty much at its beginning.

Keywords: graph, conjecture, computer-aided system, automated system, invariant, subgraph, minor.

Résumé

Les conjectures en théorie des graphes ont des formes multiples et impliquent des invariants graphiques, des classes de graphes, des sous-graphes, des mineurs et d'autres concepts dans les prémisses et/ou conclusions. Divers critères abstraits ont été proposés afin de trouver des conjectures intéressantes avec l'assistance de l'ordinateur ou à l'aide de systèmes automatisés. A partir de l'observation que les théorèmes célèbres (et les autres) ont d'abord été des conjectures, ne fut-ce que dans l'esprit de ceux qui les ont obtenus, on passe en revue les formes qu'elles peuvent prendre. On donne également des exemples pour les formes pour lesquelles des systèmes assistés ou automatisés ont donné des résultats. Il apparait que de nombreuses formes sont inexplorées et en conséquence la recherche de conjectures assistée par ordinateur ou automatisée, malgré de nombreux succès, en est encore à ses débuts.

Mots clés: graphe, conjecture, système assisté, système automatisé, invariant, sous-graphe, mineur.

1 Introduction

"*What makes a mathematical result interesting?*" This difficult question of mathematical philosophy is seldom discussed, despite its obvious interest. Recently, needs of computer-assisted or automated systems for finding interesting new concepts, theorems or conjectures have given it some actuality, notably in graph theory. Views of several famous scientists on this topic are interspersed with discussions of graph theoretical conjectures in the large *Written on the wall* file of Fajtlowicz [50]. Colton *et al.* [32] and Larson [67], also address this question in detail.

We next mention and briefly discuss a few proposed criteria:

(a) *simplicity*: simple formulae are the most used ones, and thus the most likely to have many consequences. They also have the most potential falsifiers, as explained by Popper in his famous book "*The Logic of scientific discovery*"[76]. However, it may be hard to find many simple, new and true formulae. Moreover, some of them may be trivial, e.g., that the clique number of a graph is not larger than its chromatic number.

In a similar vein, one might suggest the two following criteria:

(b) *centrality*: conjectures should preferably involve the most central concepts of graph theory as e.g. connectedness, stability, colorability, and so forth. To illustrate, some new concepts proved to be interesting and lead to numerous results, as e.g. *pancyclicity* or having elementary cycles of all possible lengths, introduced by Bondy [10], which is close to the basic concept of cycle. This is far from being always the case for the numerous new concepts which nowadays proliferate and, to some extent, threaten the unity of graph theory.

(c) *problem solving*: instead of considering centrality in terms of concepts, one may examine it in terms of problems posed by scientists in a given field. This leads to another criterion, again stated by Popper in *"The Logic of Scientific Discovery"* [76]: "Only if it is the answer to a problem – a difficult, a fertile problem, a problem of some depth – does a truth, or a conjecture about the truth, become relevant to science. This is so in pure mathematics, and it is so in the natural sciences."

A quite different criterion is the following:

(d) *surprisingness*: Conway's answer to the question "What makes a good conjecture?" was "It should be outrageous" [50]. This means a trained mathematician finds something contrary to what suggests his well-educated intuition, and so gets a new insight. Of course, it remains to be examined whether some explanation may be found, together with new results, or the conjecture will remain an isolated curiosity.

(e) *distance between concepts* is one version of surprisingness: a conjecture will be the more interesting the farther the concepts involved are one from another. This implies an operational notion of distance, either in the conjecture-making program or possibly in a lattice of graph-theoretical concepts.

Another view comes from information theory:

(f) *information-content* relative to databases of conjectures and graphs. A conjecture is interesting if it tells more, for at least one graph than the conjunction of all other conjectures. This is the criterion of the “DALMATIAN” version of Graffiti [50], discussed in [60]. It also means the conjecture should not be redundant.

A more demanding related criterion is:

(g) *sharpness:* the conjecture should be best possible in the weak sense, i.e., sharp for some values of the parameters, or in the strong sense, i.e., sharp for all values of the parameters compatible with the existence of a graph [60].

In addition to such abstract criteria one might take a pragmatic view and say that a conjecture is interesting if it has attracted the attention of mathematicians, whoever they may be. This is fairly tautological. Note, moreover, that popularity of a result depends not only on its intrinsic merits but also on its visibility (Journal where it was published, computer systems which mention it or give access to it, as well as relations and aptitude for marketing of its author(s)).

In this paper, we follow a different approach, beginning from the observation that *well-known theorems in graph-theoretical books and papers were first conjectures, if only in the minds of those which proved them.* Instead of seeking an abstract and general criterion we more modestly try to find what forms have a number of well-known results in graph theory. On this base we reflect on what is done by available conjecture making systems, and what remains to be done.

Let us recall the definition of conjecture in Bouvier and George’s [13] *Dictionary of Mathematics*:

Conjecture: *An a priori hypothesis on the exactness or falseness of a statement of which one ignores the proof.*

As a *statement* is a very general concept in mathematics, one can expect to find conjectures of many forms. We are, as mentioned above, interested here in the various forms of graph-theoretic conjectures. We therefore make a tentative, and necessarily incomplete, catalog of such forms using books by Berge [6], Biggs [7], Bondy and Murty [12], Busacker and Saaty [20], Cvetković, Doob and Sachs [34], Haynes, Hedetniemi and Slater [61] and a few others prominent among which is Chung and Graham’s book *Erdös on Graphs* [30].

We also mention, with an example if possible, if a form has been explored by one or another system for computer-assisted or automated conjecture-making in graph theory. In accordance with the terminology of [60] we say a conjecture has been obtained *with* a system if this was done in computer-assisted mode and *by* a system if this was done in (fully) automated mode. Note that several systems can be used in either of those modes. Moreover, we mention some cases where systems, designed for other purposes, could be used for conjecture-making. As will be seen, many unexplored cases remain, most of which could apparently be explored by some enhanced version of one or another existing system.

2 Algebraic relations

2.1 General form

A first class of graph-theoretic conjectures consist in algebraic relations between graph invariants, i.e., quantities which are independent of vertices and edge labelings. Such relations may be valid for any graph G or for some particular class of graphs.

To date, this class of conjectures is the most studied, but far from the only one, in computer-assisted and automated conjecture-making, see [60] for a discussion.

Let R denote a relation and C a class of graphs; any graph G can be associated with a boolean variable, true (or equal to 1) if G belongs to this class and false (or equal to 0) otherwise [14] [16].

The general form of conjectures considered in this section can then be written

$$R \,|\, C \qquad (\text{or} \;\; C \Rightarrow R)$$

which reads:

"For any graph of class C, relation R holds".

If a relation holds for all graphs, C can be omitted.

We now review theorems and conjectures of this form, considering first R, then C, and going from the simplest to the more elaborate ones.

2.2 Linear relations and extensions

Let $G = (V, E)$ be a simple undirected graph without loops, with *order* $n = |V|$ and *size* $m = |E|$. Let $\alpha(G)$ denote the *independence number* of G, i.e., the largest number of pairwise non adjacent vertices, $\nu(G)$ the *matching number* of G, i.e., the largest number of pairwise non-incident edges, $\tau(G)$ the *vertex covering number* of G, i.e., the smallest number of vertices in a set such that each edge contains at least one of those vertices, and $\epsilon(G)$, the *edge covering number* of G, i.e., the smallest number of edges in a set such that each vertex belongs to at least one of those edges. Denote by R_1 the class of linear equalities between invariants of G.

Theorem 1 (Norman, Rabin [71], Gallai [55]) *For any graph G with matching number $\nu(G)$, edge covering number $\epsilon(G)$, vertex covering number $\tau(G)$, independence number $\alpha(G)$ and order n,*

$$\nu(G) + \epsilon(G) = n$$

and if G has no isolated vertex

$$\alpha(G) + \tau(G) = n.$$

Such equalities, valid for all graphs (or for a very large class) are rare. They are more common for particular classes of graphs. Recall that a *tree* T is a connected graph without *cycles* (paths with the last vertex equal to the first one). Let $\omega(G)$ denote the *clique number* of G, i.e., the largest number of pairwise adjacent vertices and $\chi(G)$ the *chromatic number* of G, i.e., the smallest number of colors to be assigned to the vertices of G such that no pair of adjacent vertices get the same color.

Theorem 2 (Folklore) *For any tree* T*,*

$$m = n - 1,$$

$$\omega(T) = 2$$

and

$$\chi(T) = 2.$$

Observe that coefficients of invariants in these relations are equal to 1. This need not always be the case.

Let n_1 denote the number of *pending vertices* of G, i.e., the number of vertices each belonging to a single edge. Recall the *distance* l_{ij} between a pair of vertices v_i and v_j of a graph G is the number of edges in a shortest path joining them. The *eccentricity* ecc_i of a vertex v_i is the largest distance between that vertex and another one. A *center* of G is a vertex v_i with smallest eccentricity; this eccentricity is called the *radius* of G. The *diameter* $D(G)$ of a graph G is the maximum eccentricity of its vertices, (or the largest distance between two vertices of G). The *index* (or *spectral radius*) of G is the largest eigenvalue of its *adjacency matrix* $A = (a_{ij})$, where $a_{ij} = 1$ if v_i and v_j are adjacent and 0 otherwise.

Conjecture 1 (Caporossi, Hansen [25] [24]) *For any tree* T *of size* m *and order* n *with* n_b *black and* n_w *white vertices,* $n = n_b + n_w$*, with minimum index, independence number* $\alpha(T)$*,* n_1 *pending vertices, radius* r *and diameter* $D(T)$*,*

$$2\alpha(T) - m - n_1 + 2r(T) - D(T) = 0.$$

This conjecture, obtained by AGX, is open. It is unlikely that an equality conjecture with as many invariants could be found by hand. Note that coefficients of invariants are small integers. AGX can also obtain conjectures with real numbers (approximated to a reasonable extent, as computations are made by machine).

Let d_j, for $j = 1, 2, .., n$, denote the *degree* of vertex v_j,i.e., the number of edges incident with v_j. Recall that the *Randic index* [79] of a graph $G = (V, E)$ is defined by

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

and the irregularity $irr(G)$ [1] of G by

$$irr(G) = \sum_{(i,j)/\{v_i,v_j\}\in E} |d_i - d_j|.$$

Conjecture 2 *For any tree T of size m with maximum degree $\Delta \leq 3$ and maximum irregularity $irr(T)$, Randic index $Ra(T)$, and n_1 pending vertices,*

$$Ra(T) = -0.027421\, irr(T) + 0.538005\, m - 0.1104848\, n_1 + 0.614014.$$

This conjecture is proved in the Appendix. Extremal trees have vertices of degree 3 and 1 alternatingly, as far as possible. Note that the system GRAPH [33] [35] could also have been used to find such extremal trees interactively, and, after characterizing them, possibly lead to the above result.

Linear inequalities form a class R_2 of relations and are more common in graph theory than linear equalities. Let $\chi'(G)$ denote the *edge-chromatic number* (or chromatic index) of G, i.e., the smallest number of colors needed to color the edges of G such that no two incident edges have the same color.

Theorem 3 (Vizing [85]) *For any graph G with maximum degree Δ and chromatic index $\chi'(G)$*

$$\Delta \leq \chi'(G) \leq \Delta + 1.$$

Many linear inequality conjectures have been obtained by several systems, and proved, refuted or remain open. We mention a few. Let $\bar{l}(G)$ denote the average distance between pairs of vertices of G.

Conjecture 3 (Graffiti 2, Fajtlowicz [50]) *For any connected graph G with average distance $\bar{l}(G)$ and independence number $\alpha(G)$,*

$$\bar{l}(G) \leq \alpha(G).$$

Conjecture 4 (Graffiti 3, Fajtlowicz [50]) *For any connected graph G with average distance $\bar{l}(G)$ and Randic index $Ra(G)$,*

$$\bar{l}(G) \leq Ra(G).$$

Both conjectures were obtained with Graffiti; the former was proved by Chung [29] and the latter is open.

A *chemical graph G* has maximum degree 4 (due to the valency of carbon).

Conjecture 5 (Caporossi, Hansen [25] [24]) *For any chemical graph G with Randic index $Ra(G)$, size m and n_1 pending vertices,*

$$Ra(G) \geq \frac{m + n_1}{4}.$$

This conjecture, obtained by AGX, was proved using arguments based on linear programming.

A shorter proof is the following. Let $G = (V, E)$ and $E = E_1 \cup E_2$ where E_1 denotes the edges of G adjacent to a leaf and E_2 those which have both endvertices of degree at least 2. $|E_2| = |E| - |E_1| = m - n_1$. Moreover, for any edge $\{v_i, v_j\} \in E_1, 1/\sqrt{d_i d_j} \geq 1/2$ as d_i and $d_j \leq 4$ and one of d_i and d_j is equal to 1, and for any edge $\{v_i, v_j\} \in E_2, 1/\sqrt{d_i d_j} \geq 1/4$. Hence, $Ra(G) \geq (m - n_1)/4 + n_1/2 = (m + n_1)/4$. □

A third class of relations, R_3, is obtained by using floor and ceiling operators.

Let $\gamma(G)$ denote the *domination number* of G (or *exterior stability number*), i.e., the smallest number of vertices in a set such that any vertex not in the set is adjacent to one in the set; let $g(G)$, the *girth* of G denote the length of the smallest cycle of G.

Theorem 4 (Brigham, Dutton [15]) *For any graph G with minimum degree $\delta \geq 2$ and girth $g(G) \geq 5$,*

$$\gamma(G) \leq \left\lceil \frac{n - \lfloor g(G)/3 \rfloor}{2} \right\rceil .$$

Not much has been done regarding the use of the operators $\lfloor a \rfloor$ (floor of a, or largest integer not larger than a) and $\lceil a \rceil$ (ceiling of a or smallest integer not smaller than a) in computer-assisted or automated conjecture-making in graph theory. Exceptions are a few conjectures obtained with Graffiti [38] and the following conjecture. Recall that the *distance polynomial* of a graph G is defined as

$$P(G) = n + mx + \sum_{k=1}^{\lfloor \frac{D(G)}{2} \rfloor} p_k x^k,$$

where p_k denotes the number of pairs of vertices v_j, v_l at distance k. Then this polynomial will be *palindromic* if

$$p_k = p_{D(G)-k} \qquad k = 0, 1, 2, .., \lfloor \frac{D(G)}{2} \rfloor.$$

and the *distance to the palindrome condition* is defined as

$$dist(G) = \sum_{k=0}^{\lfloor \frac{D(G)}{2} \rfloor} |p_{D(G)-k} - p_k|.$$

Clearly if $dist(G) = 0$ the polynomial is palindromic. AGX [22] could find trees T with a palindromic distance polynomial $P(T)$ and an even diameter $D(T)$ (finding graphs G with a palindromic distance polynomial is easy) but not with an odd diameter $D(T)$. However, its use led to

Conjecture 6 (Caporossi *et al.*[22]) *For any tree T with odd diameter $D(T)$,*

$$dist(T) \geq \lceil \frac{n}{2} \rceil.$$

This conjecture is open (and apparently hard). It was obtained interactively with AGX; however the non-automated part was easy as AGX produced trees T with odd diameter and distances $dist(T)$ equal to 5,6,6,7,7,8,8 and so forth for $n = 10$ to $n = 50$ without exception, from where the conjecture follows immediately.

2.3 Non-linear relations

A fourth class of relations, $R4$, involves powers of invariants or products of them. Usually powers are squares, cubes, inverses, square or cubic roots. Products usually involve only a pair of invariants. Recall that the *complementary graph* $\bar{G}$ of a graph G has an edge joining vertices v_i and v_j if and only if G has not.

Theorem 5 (Nordhaus, Gaddum [70]) *For any graph G of order n with chromatic number $\chi(G)$,*

$$2\sqrt{n} \;\leq\; \chi(G) + \chi(\bar{G}) \;\leq\; n+1$$

and

$$n \;\leq\; \chi(G).\chi(\bar{G}) \;\leq\; \frac{(n+1)^2}{2} = \frac{n^2}{2} + n + \frac{1}{2}.$$

Systems Graffiti and AGX led to several conjectures with powers or products of invariants. Define [50] the temperature t_j of vertex v_j of G as

$$t_j = \frac{d_j}{n-d_j} \;\; j = 1, 2, .., n.$$

Conjecture 7 (Graffiti 834, Fajtlowicz [50]) *For any connected graph G with average distance $\bar{l}(G)$ and temperature of vertices of the complementary graph $t_j(\bar{G})$, $j = 1, \ldots n$,*

$$\bar{l}(G) \leq 1 + \max_j \; t_j(\bar{G}).$$

This conjecture could be reformulated as

$$(1 + \delta(G))\,\bar{l}(G) \leq n,$$

and was refuted by AGX [26]; the counter-example consists of two triangles joined by a path with seven edges. A weaker, but simple and elegant, conjecture is the following:

Conjecture 8 (Graffiti 127, Fajtlowicz [50]) *For any connected graph G*

$$\delta(G).\bar{l}(G) \leq n.$$

After this conjecture remained open for more than 10 years, a stronger result, implying it as a corollary, was obtained by Beezer *et al.* [5].

The *energy* E of a graph G can be defined [57] [56] as

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

where the λ_i , $i = 1, 2, \ldots, n$ are the eigenvalues of the adjacency matrix $A(G)$ of G.

Conjecture 9 (Caporossi *et al.* [21]) *For any graph G,*

$$E \geq 2\sqrt{m}$$

and

$$E \geq \frac{4m}{n}.$$

Both relations, obtained with AGX, could easily be proved.

A fifth, rare, class of relations, R_5, involve exponentials or logarithms.

Theorem 6 (Berge [6]) *For any connected graph G with a maximum degree $\Delta \geq 2$ and radius $r(G)$,*

$$r(G) \;\geq\; \frac{log(n\,\Delta - n + 1)}{log(\Delta)}$$

A few other conjectures involving logarithms were recently obtained with Graffiti [38].

Let $\rho(G)$ denote the *path covering number* of G, i.e., the smallest number of vertex disjoint paths needed to cover all vertices of G.

Conjecture 10 and 11 (De La Vina *et al.* [38]) *For any graph G with independence number $\alpha(G)$, radius $r(G)$ and path covering number $\rho(G)$,*

$$\alpha(G) \geq r(G) + ln(\rho(G))$$

and

$$\alpha(G) \geq ln(r(G)) + \rho(G).$$

These conjectures are open.

2.4 Qualitative relations

Relations of another form, i.e., *qualitative* ones, define class R_6. They are rarely used in graph theory but quite frequent in other fields such as economics [81], particularly in *comparative statics*. Qualitative relations describe trends of invariants. e.g:

"invariant i_1 increases when invariant i_2 increases"

or

"invariant i_1 decreases when invariant i_2 increases",

which may be expressed by

$$\frac{\Delta i_1}{\Delta i_2} > 0 \qquad \text{and} \qquad \frac{\Delta i_1}{\Delta i_2} < 0$$

respectively, where Δi_2 is an increase in invariant i_2 and Δi_1 the corresponding change in the invariant i_1.

A tree with n vertices is bipartite and its vertices can be colored, say, in black and white; let n_b and n_w denote the numbers of black and of white vertices respectively (with $n_b + n_w = n$). In [37] color-constrained trees, i.e., trees with fixed n and $n_b \geq n_w$, and with minimum index are studied. This led to the following result:

Conjecture 12 (Cvetković *et al.* [37]) *For all trees T with n vertices, n_b black ones and n_w white ones, $n_b \geq n_w$, the minimum value of the index λ_1 (T) increases monotonously with $n_b - n_w$.*

This qualitative conjecture was obtained with AGX and is proved in the cited reference.

2.5 Conditions

We next discuss the classes C of graphs G which are the most used in conjectures of the type $R|C$. Several of them have already been illustrated by examples given above.

A first class, C_1, is composed of *conditions necessary for the invariants $i_1, i_2, ...$ used in the relation R to be defined*. Quite often the graph will have to be *connected*, i.e., any two vertices must be joined by a path.

Examples are conjectures 3,4,7 and 8 above where connectedness is needed for average distance not to be infinite. In other conjectures, such as those on trees, e.g. conjecture 6 above, connectedness is implicit, as a tree is a connected graph without cycles.

Another class C_2 consists of *conditions eliminating trivial cases.* An example is that there should be no isolated points, i.e., the minimum degree $\delta(G) \geq 1$. This is illustrated by the second formula of Gallai's theorem (Theorem 1 above).

Forbidden subgraphs can also be used to obtain well-known classes of graphs, which we denote collectively by C_3.

A first case is *triangle-free* graphs.

Theorem 7 (Fraughnaugh, Locke [54]) *For any connected triangle-free 3-regular graph G with independence number $\alpha(G)$ and order n,*

$$\frac{\alpha(G)}{n} \geq \frac{11}{30} - \frac{2}{15n} \qquad \left(or\ \alpha(G) \geq \frac{11}{30}n - \frac{2}{15} \right)$$

Conjecture 13 (Graffiti 116, Fajtlowicz [50]) *For any triangle-free graph G with index $\lambda_1(G)$ and Randić index $Ra(G)$,*

$$\lambda_1(G) \leq Ra(G).$$

This has been proved by Favaron, Mahéo and Saclé [51].

A generalization is to consider graphs without odd cycles C_{2k+1} for all positive integers k, i.e., *bipartite graphs.*

Theorem 8 (König [64]) *For any bipartite graph G with matching number $\nu(G)$ and vertex covering number $\tau(G)$,*

$$\nu(G) = \tau(G).$$

A more drastic condition is to exclude all cycles, which of course gives trees, if connectivity is assumed, and *forests* otherwise.

Conjecture 1 above does not hold for all trees; the following one does

Conjecture 14 (Caporossi, Hansen [25] [24]) *For any tree T,*

$$\alpha(T) \leq \frac{1}{2}(m + n_1 + D(T) - 2r(T))$$

and

$$\alpha(T) \geq \frac{1}{2}(m + n_1 + D(T) - 2r(T) - [\frac{n-2}{2}]).$$

Symbols are defined above. Both relations were found with AGX; the former is proved in [25] and the latter in [24].

A generalization consists in defining a new class C_4, in terms of excluded subgraphs of G obtained by applying some operations. A first such operation is an homomorphism, i.e., removal of degree 2 vertices: if $d_j = 2$ and the neighbors of v_j are v_i, v_k, remove v_j and replace its two incident edges by an edge joining v_i and v_k. Then G is *planar* if it contains no induced subgraph homomorphic to K_5 or $K_{3,3}$ (see below).

Theorem 9 (the four-color theorem, Appel, Haken [2] [3] [4])
If G is planar and has chromatic number $\chi(G)$ then

$$\chi(G) \leq 4.$$

This result was conjectured already in 1852 and was proved in 1976, with important computer aid; see also the more recent and shorter, but still computer-aided proof of Robertson *et al.* [80].

3 Conditions for belonging to a class of graphs

A second class of graph theoretic conjectures consists in necessary and/or sufficient conditions, expressed as algebraic relations, for a graph G to belong to a particular class C. Sufficient conditions appear most often. Their general form is

$$C \Leftarrow R$$

which reads:

"For any graph G, relation R implies G belongs to class C".

Necessary conditions have the form discussed in section 2, i.e., $C \Rightarrow R$. In rare cases, necessary and sufficient conditions are available: $C \Leftrightarrow R$. One can have also conditions valid only for some classes of graphs, e.g. $(C_1 \Leftarrow R) \mid C_2$. Recall that a graph is *Hamiltonian* if and only if there exists a cycle of G going once and only once through each vertex.

Theorem 10 *A graph G of order $n \geq 3$ with degree sequence $d_1 \leq d_2 \leq \ldots d_n$ is Hamiltonian if one of the following conditions holds:*
(i) (Dirac [40]) $d_k \geq \frac{n}{2}$ for all $k = 1, 2, \ldots n$;
(ii) (Ore [72] $d_u + d_v \geq n$ for all pairs of non adjacent vertices u,v;
(iii) (Pósa [77]) $d_k > k$ for all k with $1 \leq k \leq \frac{n}{2}$;
(iv) (Bondy [9]) $d_j + d_k \geq n$ for all j, k with $d_j \leq j, d_k \leq k - 1$.

Instead of a single relation R, one could have a conjunction or a disjunction of relations (as shown in the previous theorem, when the four conditions are taken jointly) or some more complicated logical combination of relations.

Relations of this form do not appear to have been much studied with computer-assisted or automated conjecture-making systems. One possible approach would be to consider conjectures which have not yet been refuted or proved, for some class C of graphs and test, on a database of examples or with an optimization routine, if one or several of them appear to be sufficient for G to belong to C.

Another approach would be to study conjectures valid for critical graphs related to the property defining C (*i.e.,* graphs G belonging to class C but who cease to be so if a vertex or an edge is removed), then to see if these conjectures hold for all graphs of C, or can be modified for this to be the case.

4 Inclusions between classes of graphs

A third class of graph-theoretic conjectures describes inclusion between classes $C_1, C_2, \ldots$ of graphs. The simplest form is then

$$C_1 \subseteq C_2$$

or, in rare cases,

$$C_1 \equiv C_2$$

which read

"All graphs of class C_1 belong to class C_2"

e.g.

"All trees are bipartite graphs"

and

"A graph belongs to class C_1 if and only if it belongs to class C_2"

e.g.

"A tree is a connected graph without cycles"

(this is sometimes taken as a definition but one can also use the following one: "A tree is a connected graph with $n-1$ edges").

Definitions of classes can be more general, *e.g.,* correspond to boolean expressions on simple classes of graphs or subgraphs in G, or possibly some graph derived from G by transformation such as removing vertices of degree 2.

Theorem 11 (Kuratowski [65]) *A graph G is planar if and only if it does not contain an induced subgraph homeomorphic to K_5 or $K_{3,3}$.*

The system *Graph Theorist* developed by Epstein [42] [43] [44] [45] represents classes of graphs by constructive definitions, *i.e.,* properties are associated with the classes of graphs satisfying them and algorithms are specified to construct (at least in principle) all graphs of these classes. Then inclusion among classes is studied leading to conjectures and their proof.

Such conjectures seldom appear to be new, the aim of Graph Theorist being more to understand mathematical reasoning than derive new results.

Relations of the above form do not appear to have been studied with other conjecture-making systems in graph theory.

5 Implications between relations

A further class of conjectures relates to implications and equivalences between relations $R_1, R_2, \ldots$, *i.e.,* they are of the form

$$R_1 \Rightarrow R_2$$

or

$$R_1 \Leftrightarrow R_2$$

Again these forms may be generalized to consider conjunctions, disjunctions or more complex logical expressions of several relations.

These forms are basic in mathematics and graph theory. They correspond to several problems:

5.1 Corollaries

The conjecture is then that corollary R_2 is a consequence of theorem R_1.

Conjecture 15 *The lower bound (*Berge *[6]) on the independence number $\alpha(G)$ of any graph G of order n and size m*

$$\alpha(G) \geq \frac{n^2}{2m+n}$$

is implied by the lower bound (Favaron *et al.* [52])

$$\alpha(G) \geq \left\lceil \frac{2n - \frac{2m}{\lceil \frac{2m}{n} \rceil}}{\lceil \frac{2m}{n} \rceil + 1} \right\rceil .$$

This is indeed the case, the latter bound being best possible for all n and m compatible with the existence of a simple graph.

Conjecture 16 [52] *The second relation in Conjecture 15 is equivalent to the following one (proposed earlier in* [59]*):*

$$\alpha(G) \geq \left\lceil n - \frac{2m}{1 + \lfloor \frac{2m}{n} \rfloor} \right\rceil + \left\lceil \frac{n - \lceil n - 2m/(1 + \lfloor \frac{2m}{n} \rfloor)(1 + \lfloor \frac{2m}{n} \rfloor) \rceil}{2 + \lfloor \frac{2m}{n} \rfloor} \right\rceil .$$

This conjecture is correct (but stated without proof in [52]).

Corroborating, refuting or strengthening conjectures such as the two last ones can be done in several ways:
(i) enumerating small graphs with systems such as Nauty or geng [69];
(ii) building interactively a counter-example, with a system such as GRAPH [33] [36];
(iii) minimizing the difference between the right hand-sides of both conjectures with AGX while parametrizing on n and m [21] [24].

5.2 Redundancy

If a relation R_2 is implied by a relation R_1 in a database, it may be viewed as redundant (and possibly deleted). Given R_1 and R_2, AGX is well-adapted to test a conjecture for redundancy: it will minimize (or maximize) the latter under the constraint that the former holds. This can be extended to testing a conjecture such as $R_1, R_2, \ldots R_k$ imply R_{k+1}, as well as to equivalence. However, this leads to refuting or corroborating one such conjecture not to finding it.

More generally,

> "When a new inequality relating graph invariants is discovered INGRID can be employed to determine if the same or better bounds can be obtained from previously known results" ([17] p.170).

To that effect, INGRID [17] can find among all relations of a large database if there is a small subset of them which imply a given relation. Thus given a set of relations $\Re = \{R_1, R_2, ...R_p\}$ and a relation R, INGRID discovers a statement of the form

$$R_{i_1} \cap R_{i_2} \cap \ldots R_{i_k} \;\Rightarrow\; R$$

where $k \ll p$. An example follows:

Conjecture 17 (Brigham *et al.* [17]) *The known relation between spectral radius* λ_1*, chromatic number* χ *and size* m *of a graph* G

$$\lambda_1 \leq \sqrt{2m\frac{(\chi-1)}{\chi}}$$

and

$$\chi \leq \lfloor 1 + \frac{1}{2}\sqrt{1+8m} \rfloor$$

imply the relation (Stanley [83])

$$\lambda_1 \leq -1 + \sqrt{1+8m}.$$

INGRID works as follows: it has built into it 458 relations between 37 graph invariants. The user can enter values or ranges of values for any of the invariants and INGRID then returns, using the relations, values or ranges of values for the remaining invariants. There is also a tracking function which allows the user to see the sequence of relations which led to the result, if desired.

INGRID may be used in interactive or in automated mode, i.e., in the latter case, after posing a question one just records the results in terms of values or intervals of values for invariants and of relations used.

It thus appears that the tools it uses for "helping to test the effectiveness of new theorems", as is discussed in this subsection, as well as for "helping derive theorems", which is discussed in the next subsection, are automated.

Brigham *et al.* comment as follows on the above example ([17] p.170):

> "With this insight we were able to show analytically that substitution of the second inequality into the first always produces a better bound than Stanley's except for one class of extremal graphs where they are equal. This in no way diminishes the value of Stanley's result, which gives an elegant direct relationship between λ_1 and e, but the exercise showed we need not include it in INGRID's knowledge base."

So, in this case, INGRID make a conjecture, which was later proved by hand. Observe that INGRID [17], as Graffiti's DALMATIAN heuristic ([49, p. 370]), does not include a relation in its database of relation if it is not informative. In the former case, this means it is implied by the union of all previous ones and in the latter case that this is true for the restricted set of graphs in the database of examples.

5.3 Paths towards new relations

The conjecture making function of INGRID just described can be extended to help finding new relations. Indeed, "INGRID does not of itself find new theorems relating graph invariants, but it can be a valuable tool in aiding a researcher to do just that" ([17] p.170). Assuming an unknown but interesting relation exists between two invariants i_1 and i_2, one may vary one of them, observe the influence on the bounds of the other and use the tracking function to see which relations (implying quite different invariants than i_1 and i_2) are invoked by the system in computing these bounds. This leads to a conjecture of the form

"Relations $R_1, R_2, \dots R_k$ in the database lead to a relation between invariants i_1 and i_2."

Then algebraic manipulations can be used to derive this relation, as illustrated by the next example:

Conjecture 18 (Brigham *et al.* [17]) *The relations*

$$\Delta \leq \lambda_1^2,$$

$$\nu \geq \frac{n}{\Delta - 1},$$

$$\epsilon \leq n - \nu$$

and

$$\theta_0 \leq \alpha$$

where the symbols are described above, except for the clique cover number $\theta_0 = \chi(\bar{G})$, imply relation(s) between λ and θ_0.
This indeed led to the relations

$$\theta_0 \leq n[\lambda_1^2/(1 + \lambda_1^2)]$$

and

$$\theta_0 \leq \frac{1}{2} + [n(n-1) - \lambda_1(\lambda_1 - 1) + \frac{1}{4}]^2,$$

which could be proved and are new.

6 Structural conjectures

Many theorems in graph theory specify partially or completely the structure of some classes of graphs. In particular extremal graphs, *i.e.,* graphs for which an invariant takes its minimum or maximum value have been much studied, as shown in Bollobas' book [8] on that topic. Critical graphs have also received much attention.

Theorem 12 (Turan [84]): *If G is a graph of order n with independence number $\alpha(G)$, and minimum number of edges, then G is isomorphic to the graph $G_{n,k}$ composed of k disjoint cliques, r of which have q vertices and the others $k-r$ of which have $q-1$ vertices, where r and q are such that $n = q(k-1) + r$.*

This result has been generalized in many ways.

The energy of a graph has been defined above, and two lower bounds in terms of m and n given.

Conjecture 19: *For any graph G with energy $E(G)$, and size m the bound*

$$E(G) \geq 2\sqrt{m}$$

is attained if and only if G is complete bipartite.

This conjecture obtained with AGX, is proved in [21].

The Randic index of a graph has also been defined above.

Conjecture 20: *For any chemical tree T (with a maximum degree 4) of given size m, the Randic index is minimum if and only if it belongs to one of the three families represented in Figure 1 or is obtained from such a tree by iterated removal of three pending edges incident with a same vertex and their addition at another pending vertex.*

This conjecture, obtained with AGX, is proved in [23].

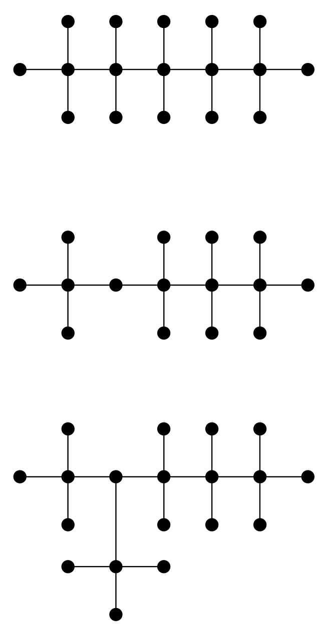
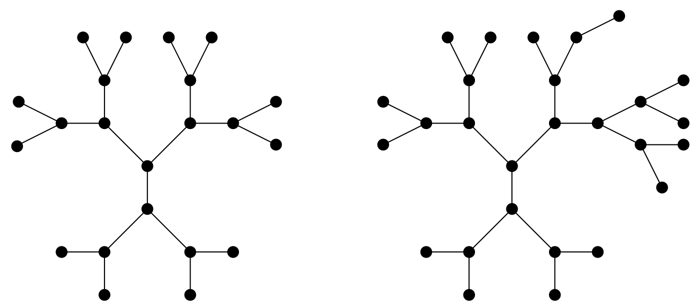


Figure 1: Three classes of chemical trees with minimum Randic index.

Dendrimers [41] are trees with a given maximum degree Δ which are as regular as possible (*i.e.,* regular except for pending vertices) and symmetric around one central vertex (see Figure 2a). It has long been surmised that:

Conjecture 21: [62] [63] *Dendrimers have minimum Wiener index (or total distance between pairs of vertices) among all trees with maximum degree Δ and the same order n.*



(a) (b)

Figure 2: Dendrimers without and with additional edges.

AGX has corroborated this conjecture, and led to observe that if the number of edges does not correspond to that one of a dendrimer, additional edges should be as close as possible (see Figure 2b). This conjecture was recently proved, independently by Fischermann *et al.* [53] and by Zheng [86].

7 Counting and Enumerating

Many graph theoretic theorems give the number of graphs satisfying some specific property, often as a function of size, and sometimes provide also an implicit list of all such graphs. Another related type of problem is to find the minimum order of graphs which satisfy a given property. Computers have been extensively used in enumerative tasks from graph theory. They have led to many computer-assisted conjectures and proofs.

7.1 Counting graphs

A graph is labeled if its vertices are numbered $1, 2, \ldots n$. Two isomorphic graphs are viewed as different when their vertices are not labeled in the same way.

Theorem 13 (Cayley [27]): *There are n^{n-2} labeled trees on $n \geq 2$ vertices.*

An approach to finding conjectures of this type would be to enumerate all graphs satisfying a given property for $n = 1, 2, \ldots$ with a powerful system such as *geng* [69], then *(i)* to check if the resulting sequence of numbers is known with the Online Encyclopedia of Integer Sequences [82] ;
(ii) if not, use tools from algebra to study the sequence (and submit it to the Encyclopedia).

7.2 Enumerating graphs

Benzenoids are molecules which can be represented as planar polyhexes, *i.e.,* simply connected regions of the hexagonal lattice. They can also be viewed as graphs. Many algorithms have been proposed for enumerating polyhexes with a given number h of hexagons (see [18] for a recent survey). The first few values are given in Table 1. However, no closed form formula for these series could be found.

h	N(h)	h	N(h)	h	N(h)
1	1	9	6505	17	1751594643
2	1	10	30086	18	8553649747
3	3	11	141229	19	41892642772
4	7	12	669584	20	205714411986
5	22	13	3198256	21	1012565172403
6	81	14	15367577	22	4994807695197
7	331	15	74207910	23	24687124900540
8	1435	16	359863778	24	122238208783203

Table 1: Number of planar polyhexes ($N(h)$) according to h

Conjecture 22: *There is no closed-form formula giving the number of polyhexes with h hexagons.*

While this conjecture could be refuted, it is hard to see how to prove it.

8 Ramseyian Theorems and Conjectures

Conjectures considered up to now are expressed in terms of invariants of a graph G and structure of such a graph. Another class of results is less direct: one considers a property which must hold for all partitions of a given type defined on G, most frequently all colorings of its edges using a given number of colors. Then the effect of the imposition of this property on an invariant $i(G)$, most often its order, is studied. To illustrate let us consider all bicoloring of the edges of G. The classical Ramsey number $r(k)$ is the smallest order of a graph G such that all such bicolorings induce a K_k in G or in $\bar{G}$.

Very few Ramsey numbers are known [30], so generalized Ramsey numbers in which one considers a subgraph G_1 in G or G_2 in $\bar{G}$ have been extensively studied. Computer enumeration played an important role: in a recent version of his “Dynamic Survey” on “Small Ramsey Numbers”, Radzizowski [78] cites 71 papers which report on automated or computer-assisted determination of generalized Ramsey numbers or bounds on them. In this last case, conjectures are sometimes made on what is the most likely value.

More general questions have been asked, often by Erdös and his collaborators.

Conjecture 23 (Burr, Erdös [19]) *For every graph G on n vertices in which every subgraph has average degree at most c,*

$$r(G) \leq c'n$$

where the constraint c' depends only on n.

A conjecture of the same form for subgraphs with maximum degree Δ,

$$r(G) \leq c(\Delta)n$$

was made by the same authors and proved to hold by Chvatal *et al.* [31].

An example in which edge 3-colorings are considered is the following:

Conjecture 24 (Bondy and Erdös [11]) *Let C_p be a cycle with p vertices; then*

$$r(C_p, C_p, C_p) \leq 4p - 3.$$

Luczak [68] has shown that $r(C_p, C_p, C_p) \leq 4p + o(p)$.

Other problems concern the number of classes in a family of partition defined on a graph G.

Conjecture 24 (Erdös, Gallai, 1959 [46]) *Every connected graph on n vertices can be edge-partitioned into almost $\lfloor (n+1)/2 \rfloor$ paths.*

Instead of partitions of edges of G, one may also consider all subgraphs of G of a given type, such as, e.g. cliques. This leads to new questions, e.g.:

Problem 1 (Erdös *et al.* 1992 [47]) *Estimate the cardinality, denoted by $T(G)$, of a smallest set of vertices in G that shares some vertex with every maximal clique of G.*

While computers do not appear to have been used in the study of this problem, it seems that a specialized algorithm could prove useful.

9 Conclusions

In order to get a clear view of what are interesting conjectures in graph theory, we followed up on the observation that famous theorems in this field (as in others) were first conjectures, if only in the minds of those which proved them. This suggests a rich variety of forms. We attempted to classify them, taking into account the work done in computer-assisted or automated conjecture-making. Thus we could provide examples of a number of cases in which one or another system was successful.

Moreover, it appears that

(i) there are many classes of conjectures which have not yet been explored with or by conjecture-making systems (the more so as the present classification is exploratory and certainly not exhaustive).

(ii) different systems appear to each have their strong points and none seems presently able to obtain interesting conjectures in all the cases where the others do.

Therefore, there is much work to do, both in modifying existing systems for doing in different ways tasks done by others and expanding them to tackle new conjecture-making tasks. Clearly, while computer-assisted and automated conjecture-making is successful, the field is still at its beginning.

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Appendix. Proof of Conjecture 2

The trees with maximum degree $\Delta \leq 3$ found by *AGX* with (conjectured) maximum irregularity are represented on Figure 3.

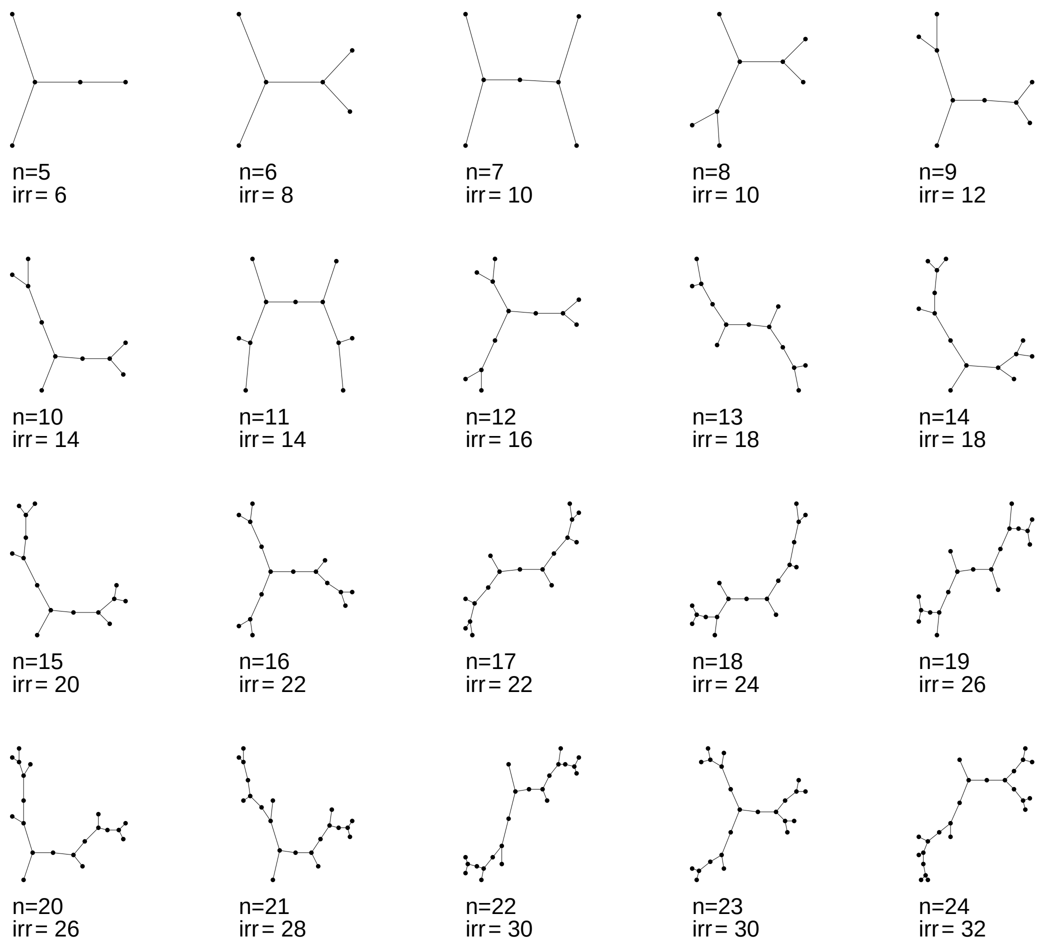

Figure 3: Extremal trees with $\Delta \leq 3$ and maximum irregularity found by *AGX*

These extremal trees are used in the following proofs, illustrating also the help provided by *AGX* in getting proofs.

Theorem 14 *For any tree T with $\Delta \leq 3$,*

$$
\begin{aligned}
irr(T) &\leq \tfrac{4n+2}{3} && \text{if } n(mod\ 3) = 1, \\
&\leq \tfrac{4n-n(mod\ 3)}{2} && \text{otherwise.}
\end{aligned}
$$

Proof. Let T be a tree with maximum degree $\Delta \leq 3$ and denote by x_{ij} the number of edges of T with endvertices of degree i and j.

By definition of the irregularity,

$$irr(T) = x_{12} + 2x_{13} + x_{23}. \tag{9.1}$$

We first solve the following system of five linear equations which holds for all trees with $\Delta \leq 3$:

$$\begin{aligned} x_{12} + x_{13} &= n_1 && (9.2)\\ x_{12} + 2x_{22} + x_{23} &= 2n_2 && (9.3)\\ x_{13} + x_{23} + 2x_{33} &= 3n_3 && (9.4)\\ n_1 + 2n_2 + 3n_3 &= 2n - 2 && (9.5)\\ n_1 + n_2 + n_3 &= n. && (9.6) \end{aligned}$$

with unkowns x_{13}, x_{23}, n_1, n_2 and n_3. That gives :

$$\begin{aligned} x_{13} &= \frac{1}{3}(n - 4x_{12} - x_{22} + x_{33} + 5) && (9.7)\\ x_{23} &= \frac{1}{3}(2n + x_{12} - 2x_{22} - 4x_{33} - 8) && (9.8)\\ n_1 &= \frac{1}{3}(n - x_{12} - x_{22} + x_{33} + 5) && (9.9)\\ n_2 &= \frac{1}{3}(n + 2x_{12} + 2x_{22} - 2x_{33} - 4) && (9.10)\\ n_3 &= \frac{1}{3}(n - x_{12} - x_{22} + x_{33} - 1). && (9.11) \end{aligned}$$

Replacing x_{13} by (9.7) and x_{23} by (9.8) in (9.1) gives

$$irr(G) = \frac{1}{3}(4n - 4x_{12} - 4x_{22} - 2x_{33} + 2) \tag{9.12}$$

which is maximal for a fixed number of vertices when the values x_{12} and x_{33} are equal to zero.

If $n(\text{mod } 3) = 1$, we can choose $x_{12} = 0$, $x_{22} = 0$ and $x_{33} = 0$ because the solutions given in Eqs. (9.7) – (9.11) are in integers. In this case, $x_{13} = (n+5)/3$, $x_{23} = (2n-8)/3$ and $irr(T) = (4n+2)/3$.

If $n(\text{mod } 3) = 0$, x_{12}, x_{22} and x_{33} cannot be all equal to zero because the solutions are no more in integers. Looking at (9.12), the best choice is to take $x_{12} = x_{22} = 0$ and $x_{33} = 1$ which is a feasible case. In this case, $irr(T) = 4n/3$.

If $n(\text{mod } 3) = 2$, there are three feasible solutions with the same irregularity value. One can choose $x_{12} = x_{22} = 0$ and $x_{33} = 2$, or $x_{12} = 1$ and $x_{22} = x_{33} = 0$, or $x_{22} = 1$ and

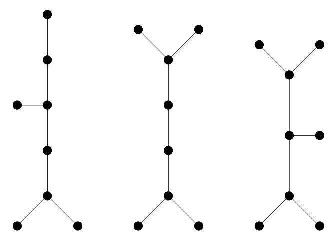

Figure 4: Three trees with maximum irregularity, $\Delta \leq 3$ and $n = 8$

$x_{12} = x_{33} = 0$. These solutions lead to $irr(T) = (4n-2)/3$. Figure 4 shows three different trees with maximum irregularity and $n = 8$. □

The graphs found by *AGX* (see Figure 3) are extremal for the irregularity by Theorem 14. The proof of this theorem gives a good characterization of these graphs in terms of x_{ij}. We now prove Conjecture 2, which was obtained automatically by *AGX* from these extremal trees.

Theorem 15 *For any tree T of size m with $\Delta \leq 3$ and maximum irregularity $irr(T)$, Randic index $Ra(T)$, and n_1 pending vertices,*

$$Ra(T) = -0.027421\ irr(T) + 0.538005\ m - 0.110484\ n_1 + 0.614014.$$

Proof. Before proceeding to the proof itself, we find which real values *AGX* has approximated. To do this, we choose 4 extremal trees given by the system (see Figure 5), compute their values for Ra, irr, m and n_1 and subsitute these values in

$$Ra = a\ irr + b\ m + c\ n_1 + d \tag{9.13}$$

where a, b, c, d are the real values sought for. For instance, the tree T_1 on Figure 5 has $Ra(T_1) = 1/\sqrt{2} + 2/\sqrt{3} + 1/\sqrt{6}$, $irr(T_1) = 6$, $m(T_1) = 4$ and $n_1(T_1) = 3$. That gives the following system of equations with unknows a, b, c and d :

$$6a + 4b + 3c + d = \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}}, \tag{9.14}$$

$$8a + 5b + 4c + d = \frac{4}{\sqrt{3}} + \frac{1}{3}, \tag{9.15}$$

$$10a + 6b + 4c + d = \frac{4}{\sqrt{3}} + \frac{2}{\sqrt{6}}, \tag{9.16}$$

$$10a + 7b + 5c + d = \frac{5}{\sqrt{3}} + \frac{2}{3}. \tag{9.17}$$

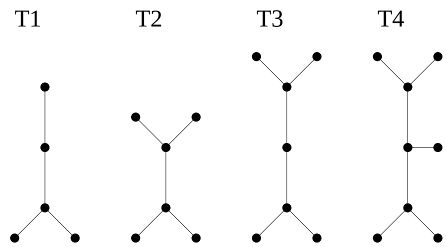

Figure 5: Four extremal trees with $\Delta \leq 3$ and maximum irregularity found by AGX

The unique solution of this system is

$$a = -\frac{\sqrt{2}}{4} + \frac{\sqrt{3}}{6} + \frac{\sqrt{6}}{12} - \frac{1}{6}, \tag{9.18}$$

$$b = \frac{\sqrt{2}}{2} - \frac{\sqrt{3}}{3} + \frac{\sqrt{6}}{6}, \tag{9.19}$$

$$c = -\frac{\sqrt{2}}{2} + \frac{2\sqrt{3}}{3} - \frac{\sqrt{6}}{2} + \frac{2}{3}, \tag{9.20}$$

$$d = \frac{3\sqrt{2}}{2} - \sqrt{3} + \frac{\sqrt{6}}{2} - 1. \tag{9.21}$$

A numerical approximation of these irrational values corresponds to the values given by AGX in the conjecture.

Let T be a tree with maximum degree $\Delta \leq 3$. We have that

$$m = x_{12} + x_{13} + x_{22} + x_{23} + x_{33}, \tag{9.22}$$

and

$$n = x_{12} + x_{13} + x_{22} + x_{23} + x_{33} + 1. \tag{9.23}$$

Moreover, by definition of the irregularity

$$irr(T) = x_{12} + 2x_{13} + x_{23}, \tag{9.24}$$

and by definition of the Randic index

$$Ra(T) = \frac{x_{12}}{\sqrt{2}} + \frac{x_{13}}{\sqrt{3}} + \frac{x_{22}}{2} + \frac{x_{23}}{\sqrt{6}} + \frac{x_{33}}{3}. \tag{9.25}$$

By Theorem 14, if $n(\text{mod } 3) = 1$,

$$x_{13} = (n+5)/3, \tag{9.26}$$

and

$$x_{12} = x_{22} = x_{33} = 0. \tag{9.27}$$

Substituting (9.27) in (9.23) and (9.23) in (9.26) gives

$$x_{23} = 2x_{13} - 6. \tag{9.28}$$

By (9.27) and (9.28), Eqs. (9.22), (9.24) and (9.25) become

$$m = 3x_{13} - 6, \tag{9.29}$$

$$irr(T) = 4x_{13} - 6, \tag{9.30}$$

and

$$Ra(T) = x_{13}\frac{\sqrt{3}+\sqrt{6}}{3} - \sqrt{6}, \tag{9.31}$$

respectively. Moreover, Eq. (9.2) gives

$$n_1 = x_{13} \tag{9.32}$$

Replace irr by (9.30), m by (9.29), n_1 by (9.32) and a, b, c, d by Eqs. (9.18) – (9.21) in the right-hand-side of (9.13) and simplify. This leads to

$$x_{13}\frac{\sqrt{3}+\sqrt{6}}{3} - \sqrt{6},$$

which is equal to the Randic index of T given by (9.32).

The other cases are similar.

If $n(\text{mod } 3) = 0$, we start with $x_{13} = (n+6)/3$, $x_{33} = 1$ and $x_{12} = x_{22} = 0$ and modify the remainder of the proof in consequence.

If $n(\text{mod } 3) = 2$ we start with the three different solutions given in Theorem 14 and apply the same ideas in each case.

□