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Variable neighborhood search for extremal graphs. 5. Three ways to automate finding conjectures

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Abstract

The AutoGraphiX system determines classes of extremal or near-extremal graphs with a variable neighborhood search heuristic. From these, conjectures may be deduced interactively. Three methods, a numerical, a geometric and an algebraic one are proposed to automate also this last step. This leads to automated deduction of previous conjectures, strengthening of a series of conjectures from Graffiti and obtention of several new conjectures, four of which are proved.

Keywords: Graph; Conjecture; Automated system

1. Introduction

As already stressed by Archimedes [5], finding conjectures and obtaining proofs are different tasks, which require different methods. Computers can help in performing both of them in graph theory. Computer-aided proofs of the four-color theorem [1–4,39] have justifiably attracted much attention (although the status of such proofs is still discussed, see e.g. [33] for a survey; note also that the recent proof [30], which uses similar techniques, of an important generalization of the four-color theorem, i.e., the Fiorini–Wilson–Fisk conjecture, shows that they are not "mathematics without posterity"). Much less attention has been paid to attempts to find conjectures in graph theory with the aid of or by computer. There have been some successes, though. Indeed, several systems for computer-aided or automated conjecture finding in graph theory have

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been developed in the last two decades. In a few cases, they led to many discoveries and numerous research papers. Such systems are based on various principles and comprise:

(i) Systems exploiting the ability of the computer to perform rapidly computations of the values of invariants (or formulae involving such invariants, which can also be viewed themselves as invariants) for series of graphs interactively modified. Such an approach is close to the initial work of a graph theorist confronted with a new problem, which it renders much more efficient. A pioneering system in this respect is "Graph", developed by Cvetković and co-workers [16–20] (this system also contains a bibliographical component [19] and an automated proving one [20]). It has led to at least 55 publications by 16 graph theorists [21].

(ii) Systems exploiting compilations of relationships between graph invariants. Such systems study classes of graphs by substituting constant or equivalent formulae for graph invariants, much as is done in constraint programming. The "Ingrid" system of Brigham and Dutton [6–9] opened up this avenue of research. Ingrid calculates possible values of graph invariants for specified classes of graphs and can provide assistance in solving practical problems (such as the design of bounded diameter communication networks), deriving new theorems by formal manipulations (an example of which is given in [9]), testing the effectiveness of new theorems, testing conjectures, resolving open problems and monitoring students of graph theory.

(iii) Systems which generate many conjectures of a simple form and then proceed to a selection of those among them which are interesting. This approach was pioneered by the system "Graffiti" developed by Fajtlowicz [23–28,33,34]. It considers formulae which are inequalities between invariants, or between an invariant and the sum of two others, and a few other such forms. These formulae are tested on a database of graphs and discarded if they are falsified by one of them or more. Possibly, other graphs are considered also and added to the database if they disprove some conjecture. Should this test be passed, it is checked whether the formulae are implied by known ones (in which case they are also discarded) and if they provide new information for at least one graph in the database, i.e., they are stronger than the conjunction of all other formulae for that graph. If not, they are provisionally set aside. If so, they are proposed to the mathematical community, on the website "Written on the wall" [29] which reports on the status of almost 1000 conjectures. Many well-known graph theorists worked on those conjectures, which led to several dozen papers [23].

(iv) Systems which enumerate rapidly all graphs of given classes, possibly exploiting symmetry. There are several such systems, the program "Nauty" [35,36] developed by McKay being a good example. They lead to conjectures if some property cannot be disproved by small counter-examples, to refutations (e.g. use of Brinkmann's [10] program for the enumeration of cubic graphs led to refutation of six of Graffiti's conjectures [38]) and to the discovery of minimal graphs with given properties and corresponding values of invariants, such as a new Folkman number [37].

(v) Systems which use some optimization tools, such as metaheuristics, to determine classes of graphs which are extremal or near extremal for some invariants or formulae under study, then deduce conjectures from interactive study of these graphs. This approach has been recently initiated by the system AutoGraphiX (AGX for short) due to the present authors [15]. In addition to suggesting conjectures, it leads to finding graphs satisfying given constraints, extremal values for various invariants of graphs subject to constraints and the corresponding classes of graphs, refutation of conjectures and suggestions for proofs.

The conjectures obtained by AGX are of three types:

(a) quantitative results, i.e., equalities or inequalities between graph invariants;
(b) qualitative results, i.e., trends of some invariants (such as increasing, decreasing, etc.) as a function of others, and
(c) structural results, i.e., characterization of extremal graphs.

AGX has been applied in [11–13,15,22] to problems of chemical graph theory and graph theory per se. In those papers, 21 conjectures were obtained (one of which turned out to be equivalent to a conjecture of Graffiti). They rank from the easy to the (apparently) very difficult. Up to now, 10 of those conjectures have been proved.

It would be of interest to automate also the procedure of finding conjectures from the graphs given by AGX, full automation of conjecture finding in mathematics being a major goal of Artificial Intelligence. Moreover, this should enhance knowledge of the little studied process of conjecture finding in graph theory, by outlining systematic methods and then testing and refining them. We address the problem in this paper and present three different approaches:

(i) A numerical approach, using the mathematics of principal component analysis, with however the aim to find what is common to all observations instead of explaining their variance.

(ii) A geometric approach, which considers extremal graphs as points in a space of characteristics, then uses a convex hull (or "gift-wrapping") algorithm to find facets, which correspond to conjectures.

(iii) An algebraic approach, which recognizes if the extremal graphs found belong to known classes, for which formulae for various invariants are available then using these to determine new relations much as in the Ingrid system [8].

These three approaches are presented and discussed in the next three sections. Most of the quantitative results previously obtained interactively with AGX could be found again in an entirely automated way by one or more of the three approaches. Moreover, five new quantitative conjectures were obtained and seven of those of Graffiti could be strengthened. Proofs of four of the new conjectures are given in the Appendix. The numerical approach has been presented previously at the XVIth IJCAI conference [14].

2. Numerical approach

2.1. Algorithm

Consider a set of m observations of n quantitative variables $x_1, x_2, \ldots, x_n$. Let $X_{m\times n} = (x_{ij})$ denote the corresponding data set. Our aim is to find a basis of all affine relations (i.e., relations of the form $a_1x_1+a_2x_2+\cdots+a_nx_n=b$, where the a_j and b are constants) satisfied by the observations. Let $\mu=(1/m)^tX1_m$ denote the vector of mean values for the columns of X. Then any affine relation between columns of X becomes a linear relation (i.e., a relation of the form $a'_1x'_1+a'_2x'_2+\cdots+a'_nx'_m=0$) between columns of $X'=X-(1^t_m\mu)$, the matrix of centered values. Furthermore, all coefficients (except b) are unchanged. Indeed if $x_1=\sum_{j=2}^n c_jx_j+d$ then

$$\mu_1=\frac{1}{m}\sum_{i=1}^m\left(\sum_{j=2}^n c_jx_{ij}+d\right)=\sum_{j=2}^n c_j\mu_j+d$$

and thus

$$x'_1=x_1-\mu_1=\sum_{j=2}^n c_jx_j+d-\left(\sum_{j=2}^n c_j\mu_j+d\right)=\sum_{j=2}^n c_jx'_j.$$

Centering variables, the first step of our algorithm, thus transforms the problem of finding affine relations into the problem of finding linear ones.

Consider then the variance–covariance matrix V defined by $V_{n\times n}={}^tX'X'$.

If the relation

$$x'_j=\sum_{\ell=1,\ell\neq j}^n c_\ell x'_\ell$$

holds, then

$$v_{jk}=\sum_{i=1}^m x'_{ij}x'_{ik}=\sum_{i=1}^m\left(\sum_{\ell=1,\ell\neq j}^n c_\ell x'_{i\ell}\right)x'_{ik}$$

$$=\sum_{\ell=1,\ell\neq j}^n c_\ell\sum_{i=1}^m x'_{i\ell}x'_{ik}=\sum_{\ell=1,\ell\neq j} c_\ell v_{\ell k}$$

which means that if a linear relation holds for the columns of X', it also holds for those of V. As V is symmetric, it still holds for its lines. The second step of our algorithm is thus to compute V.

The third and last step is to diagonalize V (with, however, some empty lines if there are relations). This can be done by Gaussian elimination. In the resulting matrix V', Dim(Im(V)) lines contain non-zero terms and correspond to independent variables. The remaining $n-$ Dim(Im(V)) lines contain only zeroes and correspond to dependent variables which may be expressed as linear combinations of the independent ones. These relations form a basis of the null-space of V. Using the initial data one can then compute the right-hand sides of the corresponding affine relations. Other forms of relations than affine ones can also be found by the proposed algorithm: to that effect, additional terms, e.g. squares and products of variables, square roots of them etc... may be computed and added to the data.

Regarding the algorithm's complexity, observe that the first step of the method, computing centered values, involves computing μ in o(mn) time and subtracting μ_j

from each x_{ij}, again in o(mn). The second step, computing the variance–covariance matrix V, takes o(mn^2) time. The third step, diagonalizing V by Gaussian elimination requires o(n^3) time. In order to avoid spurious relations, one must have $m \geqslant n$. Thus the overall complexity is in o(mn^2) (or in o(n^3) if one makes the reasonable assumption that m is o(n)). If squares and products of pairs of variables are added the complexity rises to o(n^6). Such problems, with n moderate, are still solvable in a reasonable time.

2.2. New conjectures

Vertices of a tree may be colored in black and white such that no pair of adjacent vertices have the same color. If the numbers of black and of white vertices are fixed the tree is *color-constrained*. In [22] AGX is used to study color-constrained trees extremal with respect to their index, or largest eigenvalue of their adjacency matrix. Six conjectures are obtained, and four of them proved.

To explore further the extremal trees found, values of the following 15 invariants were recorded: number n of vertices, number n_1 of pending vertices (or vertices of degree 4), number m of edges, diameter D, (maximum distance between a pair of vertices, equal to the number of edges of the shortest path joining them), radius r, (minimum over all vertices of the maximum distance to another vertex), stability number α (maximum number of pairwise non-adjacent vertices), average degree $\bar{\delta}$, average distance $\bar{l}$ (between pairs of distinct vertices), sum of distances between pairs of vertices W (or Weiner index), energy E, (sum of the absolute values of the eigenvalues of the adjacency matrix), maximum degree Δ, largest eigenvalue of the adjacency matrix λ_1, hyperwiener index WW, (sum of the squares of distances between pairs of vertices), Randić index Ra (sum over all edges of the inverse of the geometric mean of the vertices' degrees), and chromatic number χ (minimum number of colors to be assigned to the vertices such that adjacent vertices receive different colors). Note that all definitions, except those for W and WW apply to all graphs.

The algorithm was used to find a basis of affine relations on those invariants. In addition to the well-known relations $m = n - 1$ and $\chi = 2$, which are valid for all trees, the unexpected following one was obtained:

$$2\alpha - m - n_1 + 2r - D = 0,$$

and the remaining 8 invariants were proved to be linearly independent from any of the considered ones. It is unlikely that a formula with as many invariants would have been found without computer assistance.

This result can also be expressed as follows.

Conjecture 1. For all color-constrained trees with minimal index

$$\alpha = \tfrac{1}{2}(m + n_1 + D - 2r).$$

Furthermore, AGX was used to see whether this conjecture could be extended to all trees. It is not the case. However, minimizing and maximizing the left-hand side of the above equality led to the following results.

Conjecture 2. For all trees

$$\alpha \leqslant \tfrac{1}{2}(m + n_1 + D - 2r).$$

Let $\lfloor a \rfloor$ denote the largest integer smaller than or equal to a.

Conjecture 3. For all trees

$$\alpha \geqslant \frac{1}{2}\left(m + n_1 + D - 2r - \left\lfloor \frac{n-2}{2} \right\rfloor\right).$$

These two last conjectures are proved in the Appendix.

3. Geometric approach

3.1. Algorithm

Let $x_{i1}, x_{i2}, \ldots x_{ip}$ denote the values of selected graph invariants for graphs G_i, $i = 1, 2, \ldots, k$ of a given class. An easy way to obtain linear conjectures on these graph invariants is to compute with "gift-wrapping" algorithm the convex hull of the corresponding points in the p-space of invariant values. Then each facet of this convex hull provides a conjecture of the form $a_1x_1 + a_2x_2 + \cdots + a_px_p \geqslant b$ where the a_j and b are constants. Such a procedure will give plausible conjectures only if

(i) all graphs of small to medium size of the class are considered; this is only possible for fairly restricted classes of graphs, or
(ii) a preliminary selection of graphs is performed; for instance AGX may be used to find graphs with extremal or near extremal values for one invariant as a function of a few others considered as parameters. This is what is done in the geometric approach algorithm.

An additional difficulty arises when relations are concave functions of some graph invariants. Linear relations will then be falsified by the first graphs larger than those used to find them. But this can easily be tested, eliminating the corresponding conjectures.
An indicator of the sharpness of the bounds obtained is the number of graphs for which they are verified as equalities. This number can be printed or represented by points in invariant space with the visual interface of AGX. The corresponding graphs can be retrieved by clicking on these points and give further insight and possibly hints on how to prove the conjecture.

3.2. New conjectures

Chemical graphs have a maximum degree of 4 (corresponding to the valency of carbon atoms). AGX was applied to find bounds on the Randić index, defined above, for such graphs. Taking the numbers n of vertices or n_1 of pending vertices and m of edges as parameters the following two conjectures were obtained:

Conjecture 4. For all chemical graphs G Randić index $\mathrm{Ra}(G)$, n_1 pending vertices and m edges

$$\mathrm{Ra}(G) \geqslant \tfrac{1}{4}(n_1 + m).$$

Conjecture 5. For all chemical graphs G with Randić index $\mathrm{Ra}(G)$, n vertices and m edges

$$\mathrm{Ra}(G) \geqslant \frac{n}{3} + \frac{m}{12}.$$

Note that these two conjectures were also obtained with the numerical approach, after keeping only observations on graphs which are local optima, i.e., such that their values of the Randić index are not above the average values of their neighbors, i.e., graphs obtained by subtracting or adding 1 to one of the parameters.

As observed in [12,13], classes of extremal graphs may depend on the parity of a parameter, or its values modulo a small number. If all extremal graphs for which a bound is attained are at regular intervals, greater than 1, for some integer parameter, further information may be obtained by removing them and iterating the procedure. This is easy to automate.

In [12], we studied the problem of finding trees with a palindromic Hosoya (or distance) polynomial. We obtained the following conjecture on distance to the palindrome condition:

Let $d(i)$ denote the number of pairs of vertices at distance i, and $d(0)$ the number of vertices of a tree T, the distance to the palindrome condition is defined as

$$d_{\mathrm{pal}}(T) = \sum_{i=0}^{\frac{D}{2}} |d(i) - d(D-i)|,$$

where D is the diameter of T.

Conjecture 6. If T is a tree with odd diameter, then

$$d_{\mathrm{pal}}(T) \geqslant \left\lceil \frac{n}{2} \right\rceil.$$

This conjecture was reproduced with the geometric approach, in two stages: the result

$$d_{\mathrm{pal}}(T) \geqslant \frac{n}{2}$$

was first obtained and the system automatically determined that it was sharp for all even n, as shown in Fig. 1. Then removing these points the system determined that

$$d_{\mathrm{pal}}(T) \geqslant \frac{n+1}{2} = \left\lceil \frac{n}{2} \right\rceil$$

for n odd, from where the conjecture $d_{\mathrm{pal}}(T) \geqslant \lceil n/2 \rceil$ follows.

In [13] trees with minimum Randić index were shown to belong to three classes according to the value of $n \bmod (3)$. Eliminating in turn extremal trees with $n \bmod (3) =$

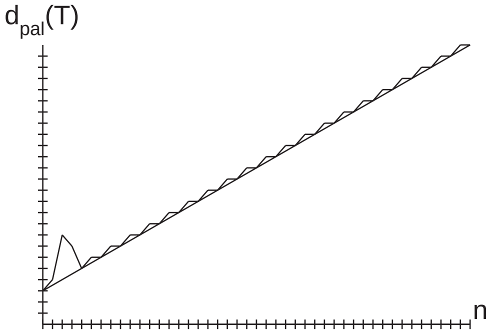

Fig. 1. Conjectured minimum distance to the palindrome condition for trees with odd diameter and $6 \leqslant n \leqslant 50$.

2 and $n \bmod (3) = 1$ led to finding again, in an automated way, the following conjecture of [13]:

Conjecture 7. Let T_n be any n-vertex chemical tree.

(a) If $n \equiv 2 \pmod 3$ and $n \geqslant 5$, then

$$\mathrm{Ra}(T_n) \geqslant \frac{5n}{12} - \frac{1}{12}$$

with equality if and only if all vertices of T_n are of degree one or four.

(b) If $n \equiv 1 \pmod 3$ and $n \geqslant 13$, then

$$\mathrm{Ra}(T_n) \geqslant \frac{5n}{12} + \frac{6\sqrt{3} - 11}{12}$$

with equality if and only if all but one vertices of T_n are of degree one or four, and the remaining vertex of degree three, is adjacent to three degree-four vertices.

(c) If $n \equiv 0 \pmod 3$ and $n \geqslant 9$, then

$$\mathrm{Ra}(T_n) \geqslant \frac{5n}{12} + \frac{2\sqrt{2} - 3}{4}$$

with equality if and only if all but one vertices of T_n are of degree one or four, and the remaining vertex, of degree two, is adjacent to two degree-four vertices.

4. Algebraic approach

4.1. Method

This third approach is closer to the way the graph theorist works, unaided by a computer, than the two first ones. Indeed, he will first draw some graphs and often try to find extremal ones. Then he will examine if they belong to a particular class and, should it be the case, study this class and derive one or more conjectures. From there, he may go on to try to prove them.

The algebraic approach comprises three steps:

(i) find extremal or near-extremal graphs for the formula under study (this can be done by AGX in the usual way);
(ii) recognize the class of graphs to which those found in (i) belong;
(iii) if a class has been found, use a compilation of relations between invariants for that class of graphs to derive new or strengthened conjectures.

A first attempt has been made to integrate part of this process within AGX. Therefore a series of rules to recognize graphs of various well-known classes (e.g. trees, stars, paths, cycles, complete graphs, regular graphs, etc.) have been included. For each class, formulae for the graph invariants discussed above and a few others as functions of n have been gathered. It appears that extremal graphs for various formulae often belong to the simplest classes, e.g. stars, paths, cycles or complete graphs. It is then possible to substitute for those graph invariants in these formulae, giving lower or upper bounds on the formulae as functions of n, which are often sharp. There may be some difficulties as extremal graphs may belong to several classes instead of a single one, as discussed at the end of the previous section. One way out is to consider the class of those graphs which correspond to local optima for the formulae. This is not without risk as the conjectures obtained may not hold for those graphs which are not used in the recognition step (an example is given below). However, once again, this may easily be checked.

4.2. Results

The method was applied to 12 conjectures among the 30 first of Graffiti [29] for which all the needed invariants were already implemented in AGX. Seven conjectures were automatically strengthened. Each time an algebraic function of n was found, it was evaluated for $5 \leqslant n \leqslant 10\,000$ to see if it takes negative values. So AGX found counterexamples to some conjectures without constructing the corresponding graphs. The smallest counterexample for Conjecture 16, a path on 26 vertices, was obtained in that way.

For this same conjecture, the strengthened conjecture was obtained by considering local optima, i.e., even values of n (see Fig. 2). It turns out not to be valid for extremal graphs with n odd (which are no more paths as for n even but path to which a pending edge is added to the penultimate vertex).

It thus appears that even a simple implementation of the algebraic approach leads to new conjectures, but these are not always correct when extremal graphs belong to several classes. Their validity can be checked on each class in turn to eliminate them automatically if they do not hold for one class at least.

The considered conjectures, their mathematical expression as well as the classes of strengthened extremal graphs found by AGX and the strengthened conjecture (if any) are given in Table 1. Note that the class of extremal graphs for Conjecture 12 was determined after selection of graphs as for Conjecture 16; Conjecture 15, was disproved using AGX in [15] and the counterexamples, i.e., even paths on more than 22 vertices, are also counterexamples to the strengthened conjecture.

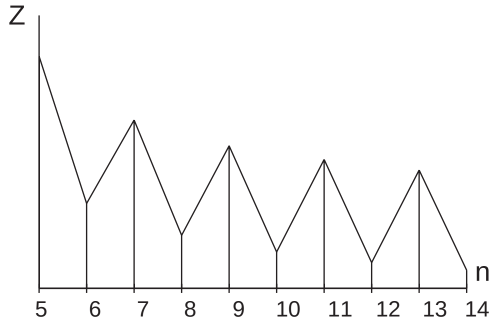

Fig. 2. Values obtained by the extremal graphs for Conjecture 16.

In Table 1, symbols have been defined before except for δ, the vector of degrees, δ_i, the degree of vertex i and d, the set of distances between pairs of distinct vertices.

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Appendix

Proof of four conjectures.

Theorem A.1 (Conjecture 2). *For all trees with stability number* α, *m edges*, n_1 *pending vertices*, *diameter D and radius r*

$$\alpha \leqslant \tfrac{1}{2}(m + n_1 + D - 2r).$$

Proof. Recall that in a tree $D = 2r$ if D is even and $D = 2r - 1$ if D is odd. Hence, $D - 2r = -(D \bmod (2))$. Assume first that D is even. Define the *star* of a vertex v_i to be the set of edges incident with v_i. Clearly, stars of vertices of a stable set are disjoint. Consider a maximum stable set S with α_1 pending vertices and α_2 inner vertices. Then, $m \geqslant \alpha_1 + 2\alpha_2 = 2\alpha - \alpha_1 \geqslant 2\alpha - n_1$ and $\alpha \leqslant \frac{1}{2}(m + n_1)$.

Assume then that D is odd. Consider a path P of length D. Either only one end vertex of P belongs to S (as defined above) and $\alpha_1 \leqslant n_1 - 1$ or there is a pair of consecutive vertices v_i and v_j of P which do not belong to S, and the edge (v_i, v_j) does not belong to the star of any vertex of S. In both cases $m \geqslant 2\alpha - n_1 + 1$ and $\alpha \leqslant \frac{1}{2}(m + n_1 - 1)$. $\square$

Table 1
Results of the use of the algebraic method to strengthen some of Graffiti's conjectures

Conjecture 2 complete graphs	$\alpha - \bar{l} \geqslant 0$ none
Conjecture 3 stars	$\mathrm{Ra} - \bar{l} \geqslant 0$ $\mathrm{Ra} - \bar{l} \geqslant \sqrt{n-1} - \frac{2}{n} + 2$
Conjecture 4 complete graphs	$\mathrm{var}(\delta) + \sum_{i \in V} \frac{1}{\delta_i} - \bar{l} \geqslant 0$ $\mathrm{var}(\delta) + \sum_{i \in V} \frac{1}{\delta_i} - \bar{l} \geqslant \frac{n}{n-1} - 1$
Conjecture 5 complete graphs	$\mathrm{mode}(d) + \sum_{i \in V} \frac{1}{\delta_i} - \bar{l} \geqslant 0$ $\mathrm{mode}(d) + \sum_{i \in V} \frac{1}{\delta_i} - \bar{l} \geqslant \frac{n}{n-1}$
Conjecture 7 stars	$r + \mathrm{Ra} - \mathrm{mode}(d) \geqslant 0$ $r + \mathrm{Ra} - \mathrm{mode}(d) \geqslant \sqrt{n-1} - 1$ if $n > 3$
Conjecture 8 stars	$\bar{l} + \mathrm{Ra} - \mathrm{mode}(d) \geqslant 0$ $\bar{l} + \mathrm{Ra} - \mathrm{mode}(d) \geqslant 2\frac{(n-1)}{n} + \sqrt{n-1} - 2$ if $n > 3$
Conjecture 12 paths	$1 + \mathrm{Ra} - r \geqslant 0$ $1 + \mathrm{Ra} - r \geqslant \frac{n-1}{2} + \sqrt{2} - \lfloor \frac{n}{2} \rfloor$ if $n > 2$
Conjecture 13 regular graphs	$\sum_{i \in V} \frac{1}{\delta_i} + \bar{l} - r \geqslant 0$ none
Conjecture 14 not recognized	$\bar{l} + \mathrm{Ra} - r \geqslant 0$ none
Conjecture 15 cycles	$\mathrm{var}(\delta) + \mathrm{Ra} - r \geqslant 0$ $\mathrm{var}(\delta) + \mathrm{Ra} - r \geqslant \frac{n}{2} - \lfloor \frac{n}{2} \rfloor$
Conjecture 16 paths	$\frac{1}{n} \sum_{j=1}^{n} \frac{\delta_j}{n-\delta_j} + \mathrm{Ra} - r \geqslant 0$ $\frac{1}{n} \sum_{j=1}^{n} \frac{\delta_j}{n-\delta_j} + \mathrm{Ra} - r \geqslant \frac{2}{n-1} + \frac{n-3}{2} + \sqrt{2} - \lfloor \frac{n}{2} \rfloor$ if $n > 2$
Conjecture 27 stars	$\mathrm{Ra} - \sqrt{\mathrm{var}(\delta)} \geqslant 0$ $\mathrm{Ra} - \sqrt{\mathrm{var}(\delta)} \geqslant \sqrt{n-1} - \sqrt{\frac{(n-3+\frac{2}{n})^2 + (n-1)(\frac{n-2}{n})^2}{n}}$

Theorem A.2 (Conjecture 3). *For all trees with stability number* α, *m edges*, *n vertices*, n_1 *pending vertices*, *diameter D and radius r*

$$\alpha \geqslant \frac{1}{2}\left(m + n_1 + D - 2r - \left\lfloor \frac{n-2}{2} \right\rfloor\right).$$

Proof. It is easy to check that the result holds for $n = 1$ and 2. Assume $n \geqslant 3$ and consider the following greedy heuristic for α. Set $S = \emptyset$; add recursively to S a pending or isolated vertex and remove the adjacent vertex (if any) and the edges of its star, but not their other end vertices. In this way a stable set with at least $\lceil n/2 \rceil$ vertices is obtained. As the set of pending vertices is stable $\alpha \geqslant n_1$; hence $\alpha \geqslant \frac{1}{2}(\lceil n/2 \rceil + n_1)$.

If n is even

$$m - \left\lfloor \frac{n-2}{2} \right\rfloor = n - 1 - \frac{n-2}{2} = \left\lceil \frac{n}{2} \right\rceil,$$

if n is odd

$$m - \left\lfloor \frac{n-2}{2} \right\rfloor = n - 1 - \frac{n-3}{2} = \frac{n+1}{2} = \left\lceil \frac{n}{2} \right\rceil.$$

Hence

$$\alpha \geqslant \left(m + n_1 - \left\lfloor \frac{n-2}{2} \right\rfloor \right).$$

As $D - 2r \leqslant 0$ the result follows. □

Recall that a chemical tree has maximum degree 4.

Theorem A.3 (Conjecture 4). *For all chemical graphs G with Randić index* $\mathrm{Ra}(G)$, *n_1 pending vertices and m edges*

$$\mathrm{Ra}(G) \geqslant \tfrac{1}{4}(n_1 + m).$$

Proof. Let n_i, $i=1,\ldots,4$ denote the numbers of vertices of degree i of G and y_{ij}, $i,j=1,\ldots,4$; $i \leqslant j$ the numbers of edges of G with end vertices of degree i and j. Then consider the 6 equations:

$$n_1 + n_2 + n_3 + n_4 = n,$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m,$$

$$y_{12} + y_{13} + y_{14} = n_1,$$

$$y_{12} + 2y_{22} + y_{23} + y_{24} = n_2,$$

$$y_{13} + y_{23} + 2y_{33} + y_{34} = n_3,$$

$$y_{14} + y_{24} + y_{34} + 2y_{44} = n_4,$$

obtained by counting vertices and degrees. These equations are clearly independent. Solving for n, n_2, n_3, n_4, y_{14} and y_{44} and substituting y_{14} and y_{44} in the objective function

$$\min \mathrm{Ra}(G) = \sum_{i=1}^{4} \sum_{j=i}^{4} \frac{1}{\sqrt{ij}} y_{ij}$$

leads to the relation

$$\begin{aligned}\min \mathrm{Ra}(G) = {} & \frac{1}{4}n_1 + \frac{1}{4}m + \left(\frac{1}{\sqrt{2}} - \frac{1}{2}\right) y_{12} + \left(\frac{1}{\sqrt{3}} - \frac{1}{2}\right) y_{13} \\ & + \frac{1}{4}\, y_{22} + \left(\frac{1}{\sqrt{6}} - \frac{1}{4}\right) y_{23} + \left(\frac{1}{2\sqrt{2}} - \frac{1}{4}\right) y_{24} \\ & + \frac{1}{12}\, y_{33} + \left(\frac{1}{2\sqrt{3}} - \frac{1}{4}\right) y_{34}.\end{aligned}$$

As $y_{12}, y_{13}, y_{22}, y_{23}, y_{24}, y_{33}$ and y_{34} are non-negative and have positive coefficients in this relation the result follows. □

Theorem A.4 (Conjecture 5). *For all chemical graph G with Randić index* Ra(G), *n vertices and m edges*

$$\mathrm{Ra}(G) \geqslant \frac{n}{3} + \frac{m}{12}.$$

Proof. The proof, being very similar to that of Theorem A.3, is omitted here. □

Note that this linear programming based type of proof, introduced in [13], is also used in [31,32] to characterize classes of chemical trees and chemical graphs extremal or near-extremal for the Randić index.

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