Toward Fully Automated Fragments of Graph Theory, II.

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Abstract. We continue the discussion of three topics initiated in the first part of this paper starting with mathematical aspects of the machine intelligence debate initiated in the books of Roger Penrose.

Stability Sorting Patterns are by-products of Minuteman, a fullerene version of Graffiti which led to the discovery of a new representation and characterization of the icosahedral C_{60}. Some of the conjectures of Minuteman postulate new properties of stable fullerenes and possibly other materials. We discuss here in greater detail two interpretations of one of the conjectures of Minuteman, one of which was incorrectly claimed to be refuted and the other one, which in spite of being refuted, presumably is approximately correct, suggesting that stable fullerenes tend to have very large separators.

Red Burton is a new implementation of Graffiti to teach mathematics Texas style, i.e., by the process of self-discovery. This version and particularly its offshoot, Little Red Riding Hood, are suitable for using the program in an almost fully automated manner.

Twas brillig, and the slighty toves
Did gyre and gimble in the wabe:
All mimsy were the borogoves.
And the mome raths outgrabe.

Through The Looking Glass

0. Introduction. This paper is the second part and an expansion of [13] which is included here for completeness and for the convenience of the readers with the customary permission of the Graph Theory Notes of New York Academy of Sciences which publishes preliminary versions of lectures presented at Graph Theory Days.

Roots of machine intelligence go back to mathematical and philosophical ideas of Descartes and to the conjecture of Hilbert known as his Tenth Problem, [4]. It took about seventy years before this conjecture was proved to be false, but meanwhile, about thirty years later, Hilbert made an even stronger conjecture which became known as his Decision Problem. This second conjecture was soon disproved independently by Gödel and Turing, but as we know today, it had a great impact on the 20th century: Turing's solution of the Decision problem led directly to the invention of computers and his paper published in "Mind" opened a heated debate on whether machines can think. Turing considered the question meaningless at the

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time, but he proposed the well-known test of how to decide this question in the future.

1. Penrose's Claim. In "Shadows of the Mind" Penrose argues that digital computers cannot have human mathematical insights. He formulated a rather technical variant of this statement and still insists on having proved it, in spite of many reservations the first of which were expressed by Putnam. A crucial point in Penrose's argument is that a digital machine could not form a mathematical belief without having a proof of its correctness, [31], [32].

In Putnam's opinion this may be an empirical issue which brings up the question how one could decide the outcome of a hypothetical experiment, [36]. The only possibility that I can think of is administering to a machine a Turing-like test asking the program to present mathematical conjectures on a given subject. I certainly do not insist that there can't be other reasonable tests, but so far nobody has suggested one to me. The correctness of conjectures would be a fairly irrelevant issue projecting more on the competence of the machine rather than on her mathematical insights.

Graffiti is a computer program for making mathematical conjectures. The author started to develop it the in mid-eighties and since then the program inspired over seventy papers. Other efforts to write conjecture-making programs are discussed in [26] and [37]. Graffiti is programmed so that whenever there is a choice, it should always take the chance of making a false conjecture rather than miss an interesting one. This comment shouldn't be construed as defensive. Fermat - perhaps the greatest conjecture-maker of all time - must have had a similar philosophy.

On one occasion two colleagues modified a conjecture of Graffiti and wrote that one could hardly expect the program to conjure their version of the problem. Yet exactly this version was already on the list of conjectures, and they published a retraction of their statement. A few years before the first chemistry results inspired by Graffiti, Professor Herbert Simon congratulated me on the response of mathematicians, but he denied the possibility that the same can be done in physical sciences. That was the first time I knew for sure that the term "discovery programs" frequently used by AI researchers was a misnomer, [28]. This attitude still persists; answering my question following his Graph Theory Day lecture, Professor Hansen made an argument in favor of similarly misleading terminology concerning conjecture-making programs and incorrectly stated that this term was used for their software by the authors of an (excellent from what I can tell) mathematical program [1].

The discussion with Professor Simon coincided with his public lecture in which he uncharacteristically made a statement about the limitation of future intelligent machines. He expressed the opinion that machine discovery can be done only by domain specific programs. The difference of our opinions on this subject is discussed in [12] in comments to conjecture 127.

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[1] Professor Hansen has acknowledged his mistake, explaining that he meant the authors of the program GRAPH, not INGRID. Still in [42] and [43], he repeats that INGRID is a conjecture-making program. The issue of what constitutes a conjecture-making program is discussed at length in [44].

Objections of this kind led me to show that the same program can make conjectures in geometry and number theory. In the latter case, it probably did not take more than an hour. Let $PR(n)$ be the graph whose vertices are numbers 2 .. n, two being adjacent if and only if they are not relatively prime. The program soon made the conjecture that η - the number of non-negative eigenvalues of this graph is equal to $\pi(n)$ - the number of primes not more than n. The conjecture was false, yet

$$\pi(n) \leq \eta$$

is true and Andrew Odlyzko confirmed later that if the difference between both sides of the inequality is not too large then this would imply the Riemann Hypothesis. The first conjecture of the geometry version was that every simple polygon contains a triangle whose vertices are selected from the vertices of the polygon. This is correct and equivalent to a known result which implies the elegant and surprising Pick's formula.

2. Concept formation problem. Lenat's papers reporting on AM and Eurisko stirred controversy with claims that these programs rediscovered Goldbach's conjecture and had the ability to invent interesting mathematical concepts demonstrated by AM's reinvention of prime numbers, [37], [26]. I will discuss the issue of inventing interesting mathematical concepts and the relevance of this question to the mathematical version of the Turing test. Unlike in the original Turing test, I do not consider it particularly interesting whether a machine could fool anyone into believing that she was a woman. This deception may be difficult to accomplish because machines may be simply superior to us in many intellectual tasks which we are not willing to concede to them yet.

Lenat's claim of AM inventing interesting mathematical concepts seems to me questionable. To start with, I do not know of any examples of simple mathematical concepts that were shown not to be interesting. Let D be the sequence of integers sorted in a non-increasing order and let D^* be the sequence obtained from D by deleting its largest term d and then subtracting 1 from the next d terms. According to the Havel-Hakimi theorem D is a graphical sequence if and only if D^* is graphical and thus iterating their reduction we end up with a sequence of zeros. The number of these zeros starting with the degree sequence of a graph G, is called the **residue** of G.

The only reason for the presence of the concept of residue in Graffiti is that at the time when I introduced it, I was short of simple easily computable invariants. Yet the conjecture that the residue is not more than the independence number resulted in four excellent papers, many more efforts, and we still do not have, in my opinion, a proof as simple as this result deserves. About a year ago, the program made the conjecture that the residue of every fullerene is at least as large as the residue of the graph induced by the complement of any of its maximal independent sets. This conjecture is now an obvious corollary, it is valid for all graphs and yet it provides a much better bound for the independence number of fullerenes. Yet, beforehand, the involved concept appears very complicated and special. The concept could be simplified by considering residues of arbitrary induced subgraphs, but then its significance might be diluted and overlooked.

3. The Dalmatian version of Graffiti, written jointly with Ermelinda DeLaVina, basically accepts a conjecture as interesting if it contributes something novel to previous conjectures. Conjectures accepted as interesting in the past may be removed from the list because of new better ones, [16]. The effect of the change of the significance of conjectures throughout the process should be even more pronounced in Red Burton, being currently developed mainly for educational purposes, though the moment I started to work on this program, it did occur to me that the only difference between the research and the educational version should be the simplicity of the initial concepts. To a degree, the invariants are also modified depending on the past performance of Graffiti. For example if the program discovers a possibility of expressing a complicated invariant in terms of simpler ones, then this invariant may be removed from the list. Sometimes, when I get interested in a conjecture, I expand the program with invariants that come to my mind pondering the problem.

We often invent, get intrigued, or even work on conjectures for their intrinsic appeal. Here is an example of such a conjecture of my own though inspired by a conjecture of Graffiti: for every prime number p, there is an arithmetic progression of p primes starting with p. The largest prime for which this is known is 13 and three such progressions were found by Holsztynski. The smallest difference found by him is 9918821194590, [12], conj. 833.

Hardly ever if at all, mathematicians invent and publish concepts for their own sake. New concepts or ideas are almost always accompanied by results, or at the very least by conjectures, but still this is perhaps the most common of all mathematical activities. When I was a student, Mycielski in defense of "concept formation" (and Marczewski's initiative of developing foundations of universal algebra) argued that every (original, I think) proof must involve a new concept. After I began to work on the program, it had occurred to me that it was exactly this role of the proof, not just correctness of results, which assures mathematics of its exceptional position among all the sciences. Otherwise Poincare would be absolutely right that "the very possibility of mathematical sciences seems an insoluble contradiction ... if all the propositions which it enunciates may be derived by rules of formal logic, how is it that mathematics is not reduced to a gigantic tautology?"

Occasionally Graffiti can be given partial credit for leading users to a novel concept. Let $e(v)$ be the number of vertices at even distance from vertex v in a connected graph G and let $h(v)$ be the number of edges whose endpoints are at the same even distance from v. Both of these invariants were in Graffiti and at one point the program made the conjecture that the independence number of every connected graph is at least as large as $\Delta(G) =$ maximum of $e(v)$ - minimum $h(v)$, [12], conj. 750.

The conjecture seemed so absurd to me that initially I was surprised that it could not be refuted just by random trial and error. Nevertheless, according to what I practiced at the time to show that it was the program, not me, that makes conjectures, the conjecture was included in [12]. The conjecture is not repeated any more, because soon after I realized that there is something to it namely that the independence number is at least the maximum of $\delta(v) = e(v) - h(v)$.

I realized the significance of the conjectured bound, after it turned out that it was one of the most handy when it was needed: together with Cvetkovic's upper bound for the independence numbers based on Cauchy's Interlacing Theorem, I could now determine enough independence numbers of higher order fullerenes to take seriously its "sorting pattern" suggesting that stable fullerenes tend to minimize their maximum independent sets. I announced this during my talk and after initial reservations expressed by Patrick Fowler, he told me later the same evening that according to his lists, the two most stable of the known fullerenes minimize their independence numbers. These two are unique fullerenes minimizing their independence numbers corresponding to their number of atoms. The δ-bound was later involved in several other stability sorting patterns discussed below. The case of equality of the δ-bound is still open.

4. Invariant Interpolation Problems. The presence of δ-bound in Graffiti is hardly sheer luck. Invention of such bounds can be perceived as the goal of the Dalmatian version. When I have a chance to include more details, I will show how the idea is related to 17th and 18th century interpolation problems, sequence continuation problems, automated construction of counterexamples and program accelerators. Invariant Interpolation Problems are informally defined in [12], but a totally unambiguous definition presents problems similarly as it is the case with the classical Interpolation Problems. The best known example of an Interpolation Problem is : define the factorial function for non-integer values of arguments. A solution is Euler's well-known Gamma function, but Hadamard proposed a different solution of this problem.

If $\Delta(G)$, rather than $\delta(G)$, performed the function described in the previous section, I would consider it reasonable to credit the program with invention of this concept. For fullerenes (particularly those that were under consideration) the difference between the two cannot be too large, so probably the Δ-bound would perform similarly as its lower case name-sake, if I had not gotten into the program's way with my own definition.

Unlike it is the case with conjectures, automated invention of mathematical concepts for their own sake does not present any difficulties, but doing this in a human-like way to accomplish a well-defined goal does. The task may be related to our innate language abilities, though almost certainly it is not as elusive as the example with $\Delta(G)$ shows. Penrose argues mainly about mathematical insights, but his main thesis is that consciousness cannot be digitally simulated. More relevant to mathematics and to the subject of this paper is the problem of simulating our language skills, [6].

I am now less skeptical than I used to be ([12], conjecture 127) about prospects of programs to invent concepts not implicit in the statement of the problem. This can be done by "knowledge transfer" - by referring to some other areas of expertise of the program, and this may be exactly how humans invent (not necessarily just mathematical) concepts. Erdös, for example, was quite interested in conjectures and number-theoretical aspects of the residue of graphs $PR(n)$, yet this concept is not implicit in number theory.

5. Stability Sorting Patterns are by-products of an interactive version of the program to view conjectures of Graffiti. To study conjectures, objects are sorted by the difference between both sides of the inequality and sometimes, when this is done for fullerene conjectures they show a conspicuous pattern by displaying the known stable examples on the top of the list and those with the largest sum of positive eigenvalues (i.e., presumed candidates for the least stable) on the bottom. One of the first such conjectures was that the separator of every fullerene is at most 1. These sorting patterns suggested that "the most stable fullerenes with a fixed number of atoms are those which are the best expanders," and I will refer to this statement here, similarly as in [11], as the stability-expanding hypothesis (SEH).

The statement should be accompanied by the caveat that there are different versions of stability and expanding properties and that though the separator is a predictor of expanding properties it is not synonymous with the concept. This list contains also my initial reaction to this finding: "Since in general, it seems that the greater the number of atoms the smaller the separator, the stability sorting pattern is unlikely to be a coincidence and thus its presence may be an indication that the stability of fullerenes (for a given number atoms) may be an increasing function of their separators." Soon after, Fowler and Rodgers computed that the stable C_{70} is 269th on the list of about 8000, 70 -atom fullerenes. In a joint paper this statement is quoted incorrectly as the hypothesis, [22]. I had not seen this version of the paper until the Spring of 2001. The only version which I received quoted their statistics as an argument against stability being an increasing function of separators. The unfortunate change was the reaction of my pointing out to Fowler that the paper should emphasize SEH. Moreover "Conjectures of Minuteman" explain that (for whatever it is worth) I wouldn't see any obvious reasons for revising SEH unless C_{60} did not turn out, contrary to my own conjecture, to be the best expander in the class of 60-atom fullerenes. The molecule has the largest separator among 60-atom molecules and the same is true for one of two stable 84-atom molecules. The second stable molecule with 84 atoms was according to the paper, "only 5th" on the list of 24 fullerenes with isolated pentagons.

This use of statistics is putting the cart in front of the horse, since the significance of SEH, as explained in [11], is exactly that it can be interpreted as a generalization of the Kroto Hypothesis according to which stable fullerenes cannot have edge-sharing pentagons [2]. According to recent preliminary computation of Craig Larson, the second stable fullerene ranks extremely high on the size of its separator on the list of over 50 000 84-atom molecules. Another argument quoted in the paper is that there is no particular chemical reason to expect a correlation between the stability and the separator. I, of course, believe that, at the very least, these two are not independent.

On one hand I always felt that SEH should be made more specific but on the other hand I had plausibility arguments indicating that the hypothesis should be valid for other materials and structures. Perhaps one can plant two trees with one seed by considering the best k-expanders for a fixed value of k, i.e., graphs that in their class maximize boundaries of various at most k-element sets of edges or vertices.

This is consistent with "local" arguments quoted in [11] as well as with the structure of single-wall nanotubes which came into the picture later. Until about

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[2] The same hypothesis was proposed independentely by Schmalz, Seitz, Klein and Hite in [38]

a half a year ago I thought of this as a Ramsey-like problem corresponding to the second of the three plausibility arguments I presented in favor of SEH at the Kalamazoo 2000 and the NanoSpace 2001 conferences, [46] . I may have now a simpler mathematical argument.

One of my plausibility arguments in favor of SEH is that the separator was proposed by Fiedler as an algebraic measure of connectivity and intuitively one should expect a positive correlation between connectivity and the stability of any reasonable kind of general structures and materials. The second argument is that a surplus of bonds inside of small clusters of atoms (making the molecule or a structure a poor expander) would have to be compensated by the presence of loosely connected pairs of clusters, creating destabilizing effects.

My third argument is that carbon nitride - a hypothetical molecule of a material harder than diamond - has girth 8 and on the average the size of its distance-induced cycles is even much larger. Good expanders, tend, of course to maximize their girth. Barry Cohen used computer modelling to generate his molecule by analogy with the density of packing of atoms of silicon nitride Si_3N_4, [1].

Another conjecture of Minuteman with a stability sorting pattern states that for any fullerene F with the independence number α

$$\alpha \leq 1 + \sum \frac{1}{\lambda^2}$$

where the summation is over non-zero eigenvalues of the Laplacian of F. The right hand side of this inequality seems to measure the energy of F, but it does it in an "exaggerated" manner compared to the sum of positive eigenvalues of the adjacency matrix of F. If this pattern, based on a small sample of Graffiti's fullerenes is correct, we may have another, hopefully more revealing, spectral predictor of stability. If this will turn out to be true, again the pattern is unlikely to be limited just to fullerenes.

One of the first fullerene conjectures of Graffiti led to a new representation and characterization of the icosahedral C_{60}: the most stable of the new carbon forms is the unique fullerene with at least 60 atoms containing a pentagonal independent set. The proof and the resulting structure suggest that the molecule may be related to Golay code.

The drawing in Figure 1 is the work of Tomaz Pisanski and Matjaz Zaversnik.

6. Stability-Separator Sorting Pattern. As explained in the previous section, in a joint paper, [22] it was stated incorrectly that C_{70} is a counterexample to SEH, the stability-expanding hypothesis [3], rather than S, [11]. The latter statement suggested the possibility that the stability of fullerenes may be an increasing function of their separators. Referring to S as hypothesis was clearly contrary to my intentions: the joint paper was written about a year after it was acknowledged in [11] (conjecture 895) that S was disproved by the data compiled by Fowler and Rodgers. It would have been pointless for me to inflate, at this stage, the status of a refuted comment, by elevating it to a hypothesis.

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[3] A new evidence in support of SEH is discussed in [44]. It appears now that stable benzenoids are also good expanders relatively to other benzenoids with the same number of atoms.

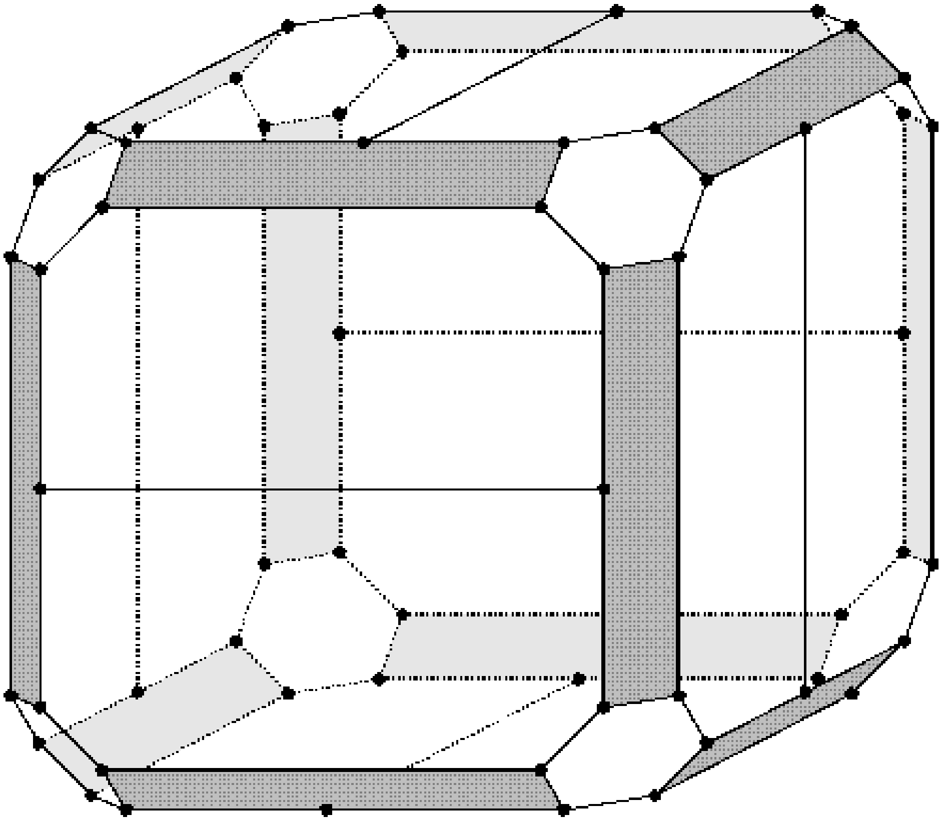

Figure 1. A Representation of Buckminsterfullerene

Before proceeding further, I will discuss shortly a related issue of the correctness of conjectures of Graffiti initiated at the '98 DIMACS meeting on Mathematical Chemistry [4] in this paper. Perhaps not surprisingly, correctness was never much of an issue before chemistry conjectures of the program [5]. In fact, quite a few of refuted conjectures of Graffiti led to interesting results by proving conjectures partially or by suggesting their modifications, as it was, for example, the case with conjecture 750 discussed here in section 3. Actually, the author of the first paper inspired by a chemistry conjecture of Graffiti stated that, in spite of "a mathematical counterexample," the chemical meaning of the refuted conjecture was basically correct, [20]. The situation with S may be similar.

It appears that a somewhat weaker interpretation of conjecture 895 is strongly supported by the data which is available to me now: the stable fullerenes tend to

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[4] This and several other issues related to this paper are discussed in comments to conjecture 127 of [12].

[5] Hilbert's Tenth and his Decision problem, proved to have negative solutions. They are referred here as conjectures, because Hilbert's formulation indicates that he was expecting positive solution in both cases.

have very large separators. However, the interpretation of data presented in [22] deemphasized the stability-separator sorting pattern arising from 895 by stressing that the second stable eighty-four atom fullerene is "only fifth" on the list of 24 isomers with isolated pentagons and ignoring that this molecule is about twentieth (according to later computations of Larson) on the list of all 84-atom fullerenes ranked by their separators. The choice of emphasizing the former statistic seems particularly arbitrary if one will take into account that the motivation for SEH (as well as its approximate, more quantitative form S) was to obtain more general and stronger conjectures than Kroto's hypothesis, which states that stable fullerenes must obey the isolated pentagon rule. Perhaps, this statistic could be justified if it had been known beforehand that the fullerenes with isolated pentagons tend to have very large separators, but this is very unlikely, since as far as I know, the study of separators and the expanding properties of fullerenes was initiated in [11]. I am not aware, and I was not given any reasons why the rank of the critical molecule in the sample of 24 fullerenes should be statistically more revealing than in the pool of about 50 000 - the number of all eighty-four atom fullerenes.

I would probably have presented a similar argument earlier, in favor of the approximate correctness of S, but I did not have access to data concerning the rank of the remaining observed fullerenes. The full information did not become available to me until Larson used Fullgen to furnish the complete data. His statistics present conspicuous evidence that the observed fullerenes tend to have very large separators; all of the eight fullerenes listed in [20] as stable, have separators overwhelmingly larger than the mean separator corresponding to their number of atoms. I would not question the choice of emphasizing only the "mathematical counterexample" rather than the statistical implications of the sorting pattern of conjecture 895, but again, the comment about the second stable fullerene being "only fifth" among 24 fullerenes with isolated pentagons presents, in my opinion, a very distorted picture of the stability-separator pattern.

Still, I appreciate that Fowler and Rodgers initiated the study of conjecture 895 and offered me examples of imposters - the term coined for some unobserved (at least, as yet) fullerenes with large separators. Of course, even if some, or even most of these imposters will never materialize as stable molecules, it is not at all an argument against the potential chemical significance of the stability-separator pattern. Most of the fullerenes with isolated pentagons have not materialized as stable molecules, yet they do not present any evidence against Kroto's hypothesis.

I also do not have any misgivings about having suggested a somewhat too strong interpretation of conjecture 895. In fact, my remark was very carefully guarded: "the stability sorting pattern is unlikely to be a coincidence and thus its presence may be an indication that the stability of fullerenes (for a given number of atoms) may be an increasing function of their separators." In any case, a counterexample may be better than a too weak conjecture, and this often is the case in Graffiti's practice: counterexamples often cause this program to invent more, rather than, as one might expect, fewer conjectures. I anticipated that, if SEH is refuted, the counterexamples may help in the discovery of more refined stability-sorting patterns, [11]. SEH is still open, but actually, counterexamples to S already performed this function.

Minuteman generated many stability-sorting patterns, but for a long time, none of them was capable of distinguishing the stable fullerenes from the imposters. Eventually I noticed that sorting patterns of the inequality from the previous section shows that stable fullerenes have larger independence number than imposters with the same number of vertices, though this sorting pattern was already present in Minuteman's conjecture 899 of [11]. Statistically this hypothesis proved to be very sound. Unexpectedly, it appears now that the independence number is one of the best, perhaps the single best known predictor of the stability of fullerenes, [42] [6].

It appears now that conjecture 895 is correct as announced during the same DIMACS workshop by Dragan Stevanovic, who proved it with the aid of the program GRAPH, written by Cvetkovic and then developed further with his collaborators, [8]. Nevertheless, even if this conjecture proved to be false, this would not affect its significance derived from its stability-separator sorting pattern. Still, since it is the correctness which is emphasized in [22], it should be pointed out that the abstract of this paper states that it presents counterexamples to conjectures of Minuteman in spite of only one conjecture being refuted, as acknowledged at the end of the paper. Moreover, the paper does not mention that one of the chemical conjectures of Minuteman, (conjecture 899) was proved before this paper was submitted for publication. Since then, two more conjectures of this program were proved to be correct by Stepanovic and Caporossi.

7. Red Burton is an implementation of the Dalmatian version of Graffiti intended initially just for educational purposes. At the same time, it was a step in the direction of a fully automated process to clearly explain the goal of the project to students. I should say at the outset, that so far this idea was barely tried and I am still at the stage of pinpointing various problems and straightening out the details. At the same time when I tried this version in two of my special problem courses, Ermelinda DeLaVina used the program for similar experiments with her students, and in Summer of 2001 she wrote a variant of the program named Graffiti.pc.

Red Burton starts with a fixed indexed set of invariants N, the leading invariant L and the sign $\geq$ or $\leq$ indicating whether conjectures are upper or lower bounds for L. One can think of these as fundamental concepts of the Red Burton (hypothetical) theory of L. If one thinks of the whole process as one program then N and L can be thought of as inputs, or preferably as input programs for evaluating invariants from N. In the case of Graffiti, this role is played by a separate program Algernon.

We will assume that we have a rule to decide for every two objects under consideration, which of them is simpler. I have experimented with several versions of simplicity and the one that I use currently is derived from a natural representation of graphs going straight back to the origin of the field. For Eulerian graphs it is simply an Eulerian tour of their edges with vertices being enumerated $1 \ldots$n. Otherwise, whenever there is a need for this, lifting of the pencil from the paper is indicated by $\bullet$. We assume that $\bullet$ is the last element in the ordering of the coding symbols.

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[6] Some recent findings seemingly supporting and providing new insight into both the stability-independence and stability-expanding hypotheses are discussed [44].

We define now $G \prec H$ if the coding sequence of G is shorter than the coding sequence of H or, in the case of equality, if this sequence is lexicographically earlier. Apart from this, Red Burton is rule-based. Runs start with one example - the simplest counterexample to the conjecture that all invariants from N are equal. There are several versions of the rules, but all of them are based on the principle that one should always provide a program with a simplest counterexample to a false conjecture or prove the "best" correct conjecture.

A sensible definition of simplicity proved to be a harder task than expected. My first choice was just lexicographic ordering, disregarding the size, but this led straight to difficulties with hypothetical theories of Red Burton. Those are very appealing questions in computational logic, but I did not see the point of complicating the picture from scratch in the classroom. It is interesting, but not unexpected, that different orderings of objects give different flavors to the subject, similarly as it is the case with Groebner bases.

The reason for the presence of coding sequences in Red Burton was however a practical necessity. The previous versions of Algernon had to be recompiled each time to communicate new examples to the program. This was an unfeasible option for classroom use and the coding sequences solved this problem. They also greatly facilitated communicating of examples electronically. Implicit in the simplicity rule is the aesthetically pleasing requirement that the user has to give priority to Eulerian counterexamples, if this is possible.

I thought of coding sequences before, wondering if graph theory would have developed differently if Euler had emphasized this, rather than his pictorial representation of graphs. My guess is that it would have, and one of the first classroom conjectures of Graffiti may be considered a confirmation of this idea. Let V be the number of vertices of a graph G, E - the number of its edges and R - the number of repetitions in the coding sequence of G. One of the first conjectures verified quickly by two class participants Tina Yang and Doug Watson, who found different proofs, was that for every Eulerian graph

$$R = E - V + 1$$

What was more important for me, I had an opportunity to tell students that the program led us to a new proof of Euler characteristic formula: drawing a plane Eulerian graph, new faces appear if and only if we encounter a repetition in the coding sequence.

One of the optional rules of Red Burton requires that for correctly conjectured inequalities, the user is supposed to determine whether the case of equality can be verified in polynomial time. Whenever this happens the conjecture is **accepted** and objects satisfying the equality are removed from the database of examples. From this point on all conjectures are interpreted as being conditional subject to the constraints that the equality does not hold true for any of the accepted conjectures. This is a solution of the problem of inventing the "right" premises for conjectures of Graffiti and the related heuristic Echo.

Most of these effects are on purpose. Usually, though not always, initial conjectures tend to be false, and counterexamples tend to be simple, conveniently leading to short coding sequences and easy exercises to practise theorem-proving skills by showing minimality of examples. Gradually difficulties increase with the number of counterexamples. The goal of the experiment is to study mathematics Texas-style, though not the traditional Texas-style. Instructors using this technique often assign as problems sequences of lemmas, leading to main results. Participants are expected to prove lemmas by themselves. There is hardly any question that the method was highly successful, at least when it was practised by R. L. Moore, but it may have some drawbacks too. One of them is the bottom-up rather than top-down approach to acquiring research experience. The responses of Red Burton to counterexamples are often refinements of refuted conjectures. It is not unusual for this version to repeat the same thesis after modification of the premises. Similar effects were clear in the first versions of Graffiti, but they began to dissipate with the growing number of invariants. This is unlikely to happen with Red Burton and particularly with its offshoot aimed at fully automating the program apart from the invention of concepts.

8. Little Red Riding Hood - a version of Red Burton - can be run, if this is the user's preference, ignoring proofs of correct conjectures. Still, as far as the students are concerned, they are presented with the challenge of acquiring or practicing their theorem-proving skills. With the right choice of initial invariants N, the method may be suitable for high-school students. In most of the interesting runs of Graffiti, each round will contain at least one false conjecture, and the user can be asked to find the simplest counterexample refuting a conjecture from the current round before proceeding to the next one. This version of the rules to run Red Burton is free of any ambiguity, and it can be implemented by a computer program.

One of the aspects of Little Red Riding Hood that appeals to me most, is that the program will be able to confirm correctness of students' solutions or warn them about their blunders without discussing them with anyone else. Actually all versions of Graffiti have this welcome aspect, but to a lesser degree; if the intended counterexample fails to accomplish its goal, then Graffiti usually repeats a supposedly refuted conjecture. Often, but not always. Little Red Riding Hood can do this always, at least in principle, because of the uniqueness of the minimal counterexamples.

The method requires quite a bit of discipline not to dismiss the program with just any counterexample, but this factor may contribute to students motivation. Otherwise the program may respond with different conjectures. If students wish to, they may run the program according to their own rules or simply by working on conjectures of their own choice, ending up with highly personalized exercises and problems. Just starting with different leading invariants may lead at once to completely different subjects, not necessarily limited to graph theory.

Once in a while it may happen that all conjectures of a given round are true. The natural interpretation of this situation - called **bingo** - is that for every object (under consideration, not just those in the database of the program) there is a conjecture made in this round such that the left and the right sides of the inequality have the same value for this object. Unless this indeed is the case, supplying the program with a counterexample to this situation will still break the stalemate and one can proceed to the next round.

Most of the interesting runs of the program will always yield at least one false conjecture in each round. This will always happen if the leading invariant L is NP-hard and all the remaining invariants from N are polynomially computable. These versions of the program will run forever modifying some of its conjectures after each round. Some of the conjectures are cyclically and some are continuously repeated in rounds providing more and more experimental evidence for their correctness. One can still end up with a correct bingo, but this would imply that $P = NP$, in which case the more appropriate term for the situation would be "big bang." Penrose does not question that in a sense a machine's insights may be superior to humans. It is not unthinkable that $P = NP$ can be proved, because machines may conjure up hundreds of novel radius, average distance, residue and δ-like bounds, constituting a valid bingo.

9. Educational and Research Experience Prospects. If I ever had doubts about the research experience potential of educational versions of Graffiti, they were quickly dispelled by the first results of Ryan Pepper, who in Spring of 2001 was attending the first fairly regular class taught Red Burton style, [33]. Though we discussed an educational use of Graffiti with DeLaVina almost from the very beginning of our collaboration, I eventually decided to try the idea after Jimmy Pritts - an undergraduate enthusiast of the Texas-style of learning - had taken with me a special course during the previous year with the idea of working exclusively on conjectures of Graffiti. Pepper's proof that the independence number of any graph is not more than its *n-residue* was the first conjecture of Graffiti, run Little Red Riding Hood style, that I could not prove out of hand.

Throughout this section, n will denote the number of vertices of a graph, α - its independence number, ω - the clique number, ρ - the residue, and ∂ - the **depth**, i.e., $n - \rho$. Let $E(\pi)$ be the sequence of terms deleted from the degree sequence π by using the Havel-Hakimi process, and let $b_j(\pi)$ be the frequency of j in E. The sequence E is called by Jelen, the **elimination sequence**, [25]. Furthermore, he defines the **k-residue** as

$$R_k(G) \equiv R_k(\pi) \equiv \frac{1}{k} \sum_{j=0}^{k-1} (k-j) \cdot b_j(\pi).$$

Jelen introduced these concepts to find a new proof and a generalization of Graffiti's conjecture,

$$\rho \leq \alpha.$$

proved first by Favaron, Mahéo and Saclé, then by Griggs and Kleitman and then again by Triesch. In Jelen's notation the residue is 1-*residue* and we have,

$$R_1 \leq R_2 ... \leq R_n.$$

Thus Graffiti conjectured and Pepper proved an upper bound analogous to one of the most interesting lower bounds for the independence discovered by the program,

$$R_1 \leq \alpha \leq R_n.$$

In response to the finding of Graffiti, Pepper almost immediately responded with several conjectures of his own. All of them turned out to be true, and they implied the conjecture of Graffiti. This led me to add new related invariants to this version of the program. Let us define the *α-residual index*, α_0, to be the smallest integer k such that the $k - residue$ is greater or equal to α. The corresponding *k-residue* will be called the **alpha-residue**.

The first conjecture that I could not prove out of hand this time, was

$$\alpha_0 \leq \alpha.$$

Let $PR(n)$ be the graph whose vertices are numbers 2 . . . n, two being adjacent if and only if they are not relatively prime. Let Λ be the *alpha-residue* of $PR(n)$, and let η be the number of non-negative eigenvalues of this graph. It would be interesting to know how close are η and Λ and, in particular, whether

$$\eta \leq \Lambda.$$

These questions may also be related to the Riemann Hypothesis, [12], conjecture 446. Startlingly, $n = 93$ is the smallest integer for which $\eta > \alpha(PR(n))$ i.e., the number of primes less or equal to n.

Concerning the *alpha-residual index* of graphs $PR(n)$, I conjecture that it tends to infinity together with n.

The version of the program that made the *n-residue* conjecture proved by Pepper was one of the first attempts to study a "conjectural theory" [7] of the independence number in terms of invariants derived from the degree sequence in a manner described in section 12, [8]. This particular choice of invariants was inspired by a question of Favaron, Mahéo and Saclé about the best lower bound for the independence number in terms of the degree sequence. At the same time I intended to use this version for educational purposes, but eventually, for that purpose, I removed from it the residual invariants, and this example is discussed in section 12. Re-running this version to document it, I noticed that one of its conjectures may be of some interest, in spite of the fact that it is easy to prove:

$$\alpha \leq 1 + \overline{\partial},$$

where $\overline{\partial} = n - \overline{\rho}$ denotes the depth of the complement of G.

Even though the last inequality is an upper bound for the independence number, this conjecture follows readily from $\rho \leq \alpha$ (because $\overline{\rho} \leq \omega$). Still, perhaps I would overlook the obvious proof if not for one of the very first conjectures of the educational version of Graffiti discussed in the class taken by Pepper and then described in his paper,

$$\alpha + \omega \leq n + 1.$$

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[7] Hardy and Wright, in their well-known textbook, refer to the twin prime conjecture as a conjectural theorem.

[8] Mathematics is exceptional in its usage of the word "theory," which in other sciences tends to refer to findings corroborated by (possibly purely mental) experiments and observations. Proofs were deliberately excluded from Little Red Riding Hood style, initially just for educational purposes, but later, to explore what seems a natural mathematical model of cognition in which the significance of statements has precedence over their correctness.

This is one of the first few clearly documented cases of a previous conjecture of Graffiti having been used as a lemma. Another such example was discussed before this paper was written in DeLaVina's [10]. Clearly the graphs satisfying the equality in $\alpha \leq 1 + \overline{\partial}$, must satisfy

$$\alpha + \omega = n + 1.$$

The inequality $\alpha + \omega \leq n + 1$ was one of the very first conjectures of Red Burton, run to find bounds for $\alpha + \omega$ in order to introduce students to Ramsey's Theorem as explained in [33], and $\alpha + \omega$ was also the first invariant used later by DeLaVina to introduce her students, including Barbara Chervenka, to educational versions of Graffiti. It was one of the very few conjectures of Red Burton (as well as previous versions of Graffiti) suited, in my opinion, for high school students. Since then, a few months before submission of this paper, I began to develop a new version of Graffiti which is seemingly capable of generating many more conjectures appropriate for high school students.

10. Jabberwocky and learning. The last statement from the previous section refers, of course, to mathematical conjectures, but there is another, already written version of Graffiti, **Jabberwocky**, suitable for high school students. Here is an example of a "conjecture" of this program. Let V be the number of vowels of a word w, L the number of letters of w, and D - the number of distinct letters of w. Then for every word w, $V \geq L - D$. In general, Jabberwocky makes conjectures about certain graphs derived from letters of words, of course not necessarily English. The vertices of the graph $G(w)$ are letters of the word, two being adjacent iff they occur in w consecutively.

I was communicating conjectures of Jabberwocky to my students mainly for the fun of it, but I had to abandon its use in the class, because it was seriously distracting students from the subject. However, Eric Westfall, a linguistics student, took with me a special course to work on conjectures of Jabberwocky about phonemes rather than letters. One purpose of Jabberwocky was to have a model of Graffiti, which could be used to explain clearly, without technical details, the underlying ideas. Another possibility, suited for student research in linguistics, is to design a Jabberwocky-based spell-checker. As pointed by Westfall, a digraph based on adjacency of phonems would be more useful for this purpose.

In the current system of education, almost at any level, research experience and learning of a subject have very little in common. I do not suggest that learning should be equated with research experience, but discouraging students from research in graduate school is a classical case of "moderation being taken to the extreme." It is not clear that the separation between the two is mandatory at any level, apart from the necessity dictated by the high student-teacher ratio which ideally would be reversed. Perhaps one will be able to remedy this situation somewhat with the design of appropriate Red Burton-like programs. Pepper's paper is one of the first case studies attempting to evaluate these prospects, and he discusses both strengths and weaknesses of the method. Other such reports were written and presented at various meetings by students of DeLaVina, starting with [5].

Both DeLaVina's and my impression is that quite a few students seem to be entertained by and some become truly fond of the method. This is reassuring, since the element of play is perhaps the single most dominating factor stimulating both the learning (whenever present) and discovery process. Initially, the interest in the method could be attributed to the curiosity about taking instructions from a computer program. Eventually, however it must have been the responsiveness, the flexibility, the unpredictability, and the full attention the machine gives to its user, that makes students enjoy the method. Still, the strongest point of Red Burton may be that (ideally) it may run synchronized with the level of the student's competence. How long this idyll lasts depends very much on the choice of the initial invariants and the definition of simplicity of objects.

Sebastian Lisken - one of the student participants of the DIMACS workshop with a strong interest in education - told me, that Red Burton appears to act in a much more human and personal manner than might be expected of a machine. Lisken was not the first person to observe that " running Graffiti is like talking to a mathematician."

Sometimes it is actually better, but it is certainly not because of the "competence" of the program. Some of the conjectures of Graffiti are better than those of many mathematicians (certainly of my own,) and they may be out of the league of some others. Talking to some of the luminaries who worked on conjectures of the program or to the beginners, who are about the only persons capable, (if they are encouraged,) of asking very naive, yet sometimes very good questions, has different rewards. Yet Graffiti was my only mathematical interlocutor, ever, who I knew for sure, did not hold back any of its "thoughts" and had the "courage," as meaningless as these words are in reference to a machine, to present any of its ideas [9]. These effects were more pronounced in the early versions of the program using few invariants and few examples, and this situation was restored in Little Red Riding Hood for exactly this purpose.

11. A Problem of Robinson. Some of the best contributions of computers to mathematics are new problems, but possibilities of implementing classical ideas available before only in principle are next in line. An example of the latter is Descartes' idea of translating "any problem in geometry" into an algebraic one and then solving it automatically. The implementation of the idea had to wait for development of symbol manipulation programs and Buchberger's algorithm which transformed algebraic geometry into an undergraduate subject.

Since most of Graffiti's conjectures are inequalities, I began to consider the possibility of extending the duality between ideals and varieties to the one between systems of polynomial inequalities and their cones. Though this was not emphasized enough before, the Dalmatian version deals with systems rather than individual inequalities.

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[9] Speaking of "thoughts" and "courage", I should mention here that similarly, as it is the case with Penrose's claims, I disagree with Searle's Chinese Room argument, but his objections concerning the significance of the Turing test, seem to me reasonable, even though they are quite a bit premature; very little progress has so far been accomplished in machine understanding of natural languages.

It was very reassuring to find out from one of my best educated colleagues John Froelich that this problem was first proposed by Abraham Robinson. To think about it, the problem may eventually have as great an impact as non-standard analysis. Still, non-standard analysis may remain forever one of the most elegant mathematical creations.

12. Little Red Riding Hood. A Case Study. Below are conjectures made in the first several first rounds of Little Red Riding Hood in the form in which they were presented to a large undergraduate graph theory class as a source of optional homework problems. The problems from this and later lists which were further simplified by limiting the set of invariants, were presented both in the class and via a mailing discussion list, one at a time, after finding the simplest counterexample in each round.

Lower Bounds for the Independence Number in terms of Degrees.

leading invariant α: independence number (lower bounds)

domain D: simple graphs.

list of invariants I : independence number and about 50 simple invariants derived from the degree sequence, including temperature and the complement of the graph, but excluding residual invariants.

style: Little Red Riding Hood, i.e., in each round of conjectures the program is informed about the unique (but note the caveat below) simplest object refuting any of the conjectures from this round.

simplicity rule for examples: simpler graphs have fewer vertices with ties being broken by the number of edges and then by lexicographic order of their degree sequences, sorted in non-increasing order. In the case of a tie at this level, it is broken by the independence number. This still may not describe uniquely the simplest object up to isomorphism, but it determines it uniquely from the view point of the program.

Symbols of Invariants.

n - number of vertices,

$d_0, d_1, d_2, ..$ - frequency of vertices of degree 0, 1, 2, etc.,

ϱ - number of vertices of different degrees.

Δ - the maximum degree and δ - the minimum degree. The degree sequence Δ_k is sorted in non-increasing order, i.e., $\Delta_1 = \Delta$ is the vertex of the largest degree, Δ_2 - the second largest, etc.

$t(v) = \frac{d}{n-d}$ - the temperature of vertex v where d is the degree of the vertex v. The maximum temperature is denoted by T, the mean by t^* and the minimum by t.

$\overline{inv}$ - the value of the invariant inv for the complement of the graph. The complement of the graph G is denoted by $\overline{G}$. The complement has the same set of vertices as G, two being adjacent iff they are not adjacent in G.

Symbols of graphs and graph operations.

k - complete graphs, p - paths, s -stars, and c - cycles. G + H denotes the disjoint union of graphs G and H, aGH - amalgamate of G and H is the graph obtained by identifying the last vertex of G with the first vertex of H. Sequences of integers are coding sequences of the graphs they represent.

Conjectures and the Simplest Counterexamples.

The numbers following the conjectured lower bounds are the **touch** numbers, i.e., the number of objects in the database of the program for which the left and the right hand sides of the inequality are equal. T - indicates that the conjecture is true, and R that it was a a conjecture refuted by the simplest counterexample, (on the same line as the corresponding conjecture.) If all conjectures in a given round are true, as in the second round, they constitute **bingo.**

In the case of bingo the example on the next line is the simplest bingo-breaker, i.e., a graph for which in neither of the proved bounds, the equality holds true.

round	conjecture(s)	touch number	status	counterexample	comments
0				k_1	
1	$\alpha = n$	1	R	k_2	
2	$\alpha \geq d_0$	1	T		eq. iff no edges
	$\alpha \geq \frac{d_1}{2}$	1	T		eq. iff $\Delta = \delta = 1$
				$k2 + k1$	bingo-breaker
3	$\alpha = \varrho$	3	R	$k_1 + k_1$	$n \geq 3$
4	$\alpha \geq d_0$	2	T		
	$\alpha \geq \varrho$	3	R	123142	
	$\alpha \geq \overline{T}$	2			$1 + \bar{t}$ is true
5	$\alpha \geq d_0$	2	T		
	$\alpha \geq \Delta_2$	2	R	$k3$	
	$\alpha \geq T$	1			
6	$\alpha = 1 + \overline{\frac{d_1}{2}}$	6	R	$c4$	
7	$\alpha \geq \overline{\frac{d_1}{2}}$	1			
	$\alpha \geq 1 + \overline{t^*}$	5			
	$\alpha \geq \varrho - 1$	1			comp 4.2

Table 1. The table of the first seven rounds of Little Red Riding Hood

The conjecture involving the mean temperature is equivalent to the inequality

$$\alpha \geq \sum_k \frac{1}{\Delta_k + 1},$$

discovered in the eighties independently by Caro and Wei. Conjectures from the second round came up in the first class taught Red Burton style, and Fred Maxwell, an undergraduate computer science student attending this course, initiated a classroom discussion leading first to a slightly better bound, namely

$$\alpha \geq d_0 + \frac{d_1}{2},$$

and then to

$$\alpha \geq d_0 + \frac{d_1}{2} + \frac{d_2}{3} + ..$$

Soon after that, Maxwell noticed that a more general pattern discovered in the class is equivalent to the Caro-Wei bound:

$$\sum_k \frac{1}{\Delta_k + 1} = d_0 + \frac{d_1}{2} + \frac{d_2}{3} + ..$$

The classroom discovery of these conjectures began with Pepper's discussion of one of the very first conjectures of Red Burton he became interested in,

$$\alpha + \omega \geq 2 + \frac{d_1}{2}$$

at a time when he did not have experience in the subject yet, [30].

The Caro-Wei result, also called the Turan bound, had previously been generalized by Favaron, Mahéo and Saclé, [19], to

$$\alpha \geq residue \geq \sum_k \frac{1}{\Delta_k + 1}.$$

Graffiti's formulation of the Caro-Wei bound, referring to the mean temperature (second conjecture of the seventh round), contains an implicit hint how to proceed with the proof, because one should expect that deletion of any vertex of the minimum temperature should not decrease the average temperature. This is closely related to the well-known fact that Maxine - the algorithm which repeatedly deletes a vertex of maximum degree, until the graph contains no edges, terminates with an independent set of size asserted by the Caro-Wei bound [10]. Maxwell's formulation on the other hand, particularly when combined with trying to prove the result by looking for a hypothetical simplest counterexample, is likely to lead a student to the discovery that MIN - the algorithm which places vertices of minimum degree into the independent set and deletes their neighbors - will also accomplish this goal. Both of these algorithms are discussed in the context of the Caro-Wei Theorem in [23].

Apart from this, one of the previous runs of the program made the conjecture,

$$\alpha \geq 1 + \bar{t},$$

which is equivalent to the familiar

$$\alpha \geq \frac{n}{\Delta + 1}.$$

The original version of Graffiti made several closely related conjectures starting with

$$\chi \geq 1 + \overline{t^*},$$

where χ is the chromatic number of the graph, [12], the conjecture with number (since it was not initially included in the list) -1.

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[10] Before the conjecture that the independence number of any graph is at least as large as the residue was proved, Shearer conjectured that every performance of Maxine terminates with an independent set at least as large as the residue, [12], conjecture 69. Comments to this conjecture contain also Shearer's elegant probabilistic argument proving the Caro-Wei bound.

In the 7th round, conjectures involving the mean temperature of the complement became too involved for the initial experience, and Little Red Riding Hood was switched to a version involving fewer and simpler invariants derived from the degree sequence. One of the first conjectures this time was,

$$\alpha \geq\ n - \epsilon,$$

where ϵ is the size of the graph. Searching for a simplest hypothetical counterexample to this conjecture, it was soon discovered in class that the graph would have to be connected, and that it would have to satisfy $n - \epsilon = 1$, which is impossible, because $\alpha \geq 1$. In the process, it became clear that trees (which were defined in the class for the first time on this occasion) could be equivalently described as connected (or acyclic) graphs with $n - 1$ edges.

The program's response to a refuted conjecture from the same round was

$$\alpha \geq n - \epsilon + \Delta - 1.$$

I had clear impression that attempts to find the simplest hypothetical counterexamples (whether they exist or not) must have helped students to appreciate the graph-theoretical cornerstone of this methodology - Kempe's attempt to prove the four-color theorem, which was about to be discussed in the class a few weeks later.

The list of conjectures displayed in the table well illustrates that a few unsophisticated examples are enough for the program to make reasonable conjectures. The pattern was present in many versions of Graffiti, and beforehand there was no reason to expect it. As a matter of fact, I still receive suggestions of expanding the program with more examples, but there is no evidence that this would improve the quality of conjectures, nor even that it would increase significantly the percentage of correct conjectures. It is actually possible that the percentage of correct conjectures would go down, since with more examples Graffiti tends to make more conjectures.

13. Automation and Understanding. There are many reasons why one might be interested in automation of the process of making mathematical conjectures, and some, basically purely philosophical, are discussed in the first section this paper. These reasons include sheer curiosity whether it is possible to do this at all, which was about all that my original interest in the problem did amount to. Other considerations, particularly in view of the conjectures of Graffiti about fullerenes and the attempt to enhance the Texas-style of teaching mathematics, are so obvious that there is not even any point in discussing them here. It is revealing though, that before the appearance of the first conjectures which had some impact outside of pure mathematics the goal of automation of the conjecture-making process was never questioned; in general, the so called *AI* debate was mainly about what computers can or cannot do, not whether they should or should not do it. However, there was one notable exception. Joseph Weizenbaum, the author of the program *Eliza* is a case of a programmer who, not without good reasons, became concerned that his program would be taken too seriously, and who became one of the first critics of controversial claims of some *AI* researchers.

Writing conjecture-making programs is an activity of interest for its own sake, and all related tasks can be considered in this context as optional. The automation of these other related activities—including proving or refuting conjectures—is irrelevant to the problem of writing such programs. There are separated branches of computer science dealing with these problems, and they are respectively called automated theorem proving and automated problem solving. After starting to work on Graffiti, it had occurred to me, that one might have a model of mathematics involving no theorem-proving at all, and soon after that, I found out that Erdös, also conjured up mathematics without proofs, [15], (see also [12], conjecture 127.) I do not know how much consideration Erdös, one of most influential conjecture-makers of all times, gave to this possibility, but Putnam (who referred to it as quasi-empirical mathematics), discussed it at length in [35] and [36]. Mycielski suggested to me even later that conjecture-making could be viewed as a search for new axioms. Indeed, stronger, not just more general, results are sometimes easier to prove. For me, the ultimate success in conjecture-making would be finding unexpected significant results which post factum are nevertheless obvious.

Similarly, whether counterexamples to false conjectures of Little Red Riding Hood are found by the program or by users is totally irrelevant to the issue of what constitutes a good conjecture. The performance of the program is of course completely determined by counterexamples, but this has only bearing on what is the “best” definition of simplicity to guarantee success, not how these unique counterexamples are found. The problem of the automation of conjecture-making processes is only superficially a programming problem. The dominating issue is the question of what makes a good conjecture. Everything else is basically a technical detail; it does not take that much programming experience to realize how difficult it may be to write a program, if a programmer has only a vague understanding of what the program is supposed to do. Working on an “algorithm” for selecting interesting conjectures is my main motivation for advocating the pursuit of full automation, because I do not know any other way of understanding what makes a good conjecture.

That is also why in the discussion of a mathematical version of the Turing test in section 1, I do not particularly care whether machines can pretend being what they are not. Authors of so-called intelligent programs tend to give more credit to machines than they deserve, perhaps committing mistakes similar to the owner of the smart horse Hans. I realize that I might not be immune to the syndrome myself, but I have always been aware of the problem, and accordingly I imposed on myself the rule of reporting all interaction with the program which I considered significant. I certainly had positive examples as guidance. Brigham and Dutton almost went out of their way to clarify possible ambiguities of what their program is not, and in particular they stated that, “Ingrid does not of itself find new theorems relating graph invariants, but it can be a valuable tool in aiding researchers to do just that.”, [2], p. 170, section 4.2.

It is generally assumed that proving theorems is always a much more difficult task then making conjectures (or for that matter inventing of problems), but it is not so at all. The thought had occurred to me at least once, well before I started to work on Graffiti. A proof of the inequality of Marcus and Lopes presented in

[13] extends to every algebraic operation of the resistance algebra $(R^+, x+y, \frac{xy}{x+y})$. Every algebraic operation f of the resistance algebra satisfies the inequality

$$f(x_1+y_1..x_n+y_n) \geq f(x_1..x_n) + f(y_1..y_n)$$

In particular, one can write a program which one by one will print an infinite sequence of theorems, which beforehand may be non-obvious to prove. Yet, it is not clear at all whether any of the resulting inequalities (apart from the one found by Marcus and Lopes) were of sufficient interest for a mathematician to have proposed them as conjectures. I am sure that there are other similar examples in the literature, and they certainly could be obtained with available symbol manipulation theorem provers.

Similarly, the main difficulty of the automation of conjecture-making processes is not a question of formal mathematics and actually, it is contrary to its spirit. As elegant and as powerful as the axiomatic approach and mathematical formalism are, they allow for solutions of problems without understanding them, and they encourage working on questions, without justifying them. Correctness of solutions in formal mathematics matters more than the significance of questions. The history of mathematics is an unrefutable testimony to the presence of a method in this madness. Working on a problem because it is appealing is an excellent reason in my opinion, though I have serious doubts that it is supposedly a well-established mathematical tradition and a right of mathematicians (even tenured ones). There are many strings attached to this supposed freedom. Many mathematicians, starting with most graduate students, work on problems because of the authority of experts or their advisors, and they do not receive much encouragement for exercising their own judgement.

Moreover, the problem of automating conjecture-making programs cannot be discussed in the framework of formal mathematics until or unless this subject will develop a counterpart to mathematical logic, dealing with the significance of mathematical statements rather than their truth. Whether this will eventually happen or not, it is a possibility hinted by a (as marginal as it is) reference to Graffiti in one of the latest versions of a thorough paper on foundations of mathematics, [28]. I consider this reference particularly encouraging in view of our perpetual debates with Mycielski of the "truth vs. significance" issue, going back to the very beginning of my work on the program.

14. Conjectures and Counterexamples. Examples generated or constructed by programs were used all the time by Graffiti. The most extensive and successful effort in this direction was made by Brewster, Dineen and Faber from Los Alamos National Laboratory who tested a number of conjectures against a database of all at most 10-element graphs. Recently, Larson used Fullgen to test stability-sorting patterns of chemical conjectures of the program. Graffiti had its own procedures for looking for counterexamples,[11] and I even attempted constructing Ramsey graphs by making conjectures about partial solutions, i.e., graphs

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[11] the first of which was Autograph, referred to in [17] - one of the earliest papers about Graffiti. Autograph was able, and I am sure still is, to find many counterexamples to conjectures of Graffiti by obvious edge-deletion and addition strategies. Later, I experimented with Ideograph, a backtracking procedure guided by constraints conjectured by Graffiti.

which could be extended to critical Ramsey graphs. I also ran Graffiti to get conjectures about critical Ramsey graphs offered to me by Radziszowski, and some of these conjectures could probably be used as reasonable heuristics in the search for Ramsey graphs, [12] conjectures 785 - 788. Later procedure *Ideograph* used some backtracking-pruning procedures of my Graffiti-preceding program *Glider*, which was able to find many $R(3,8)$-critical graphs [12].

Automating the process of finding counterexamples seemed a natural next step in the development of the program, and initially, I was taking this for granted. Still, there are many beforehand unexpected, yet now conspicuous, findings resulting from the performance of Graffiti, and one of them is that there was no need for the program to generate its own examples. The program fares quite well without them, and human-found counterexamples seem to lead to more and to more interesting theorems. Automation of finding counterexamples is of course a problem of interest for its own sake, and it is clear that many solvers of Graffiti's conjectures were using programs for this purpose. To write an efficient program of this kind may be quite a challenging problem since the most successful effort in this direction was made by the Los Alamos group who simply used for this purpose the list of all graphs with up to 10 vertices As far as Graffiti itself is concerned, many counterexamples are routinely guessed by viewing conjectures with the interactive version of Graffiti which often displays patterns directly pointing to counterexamples, in a manner similar to the one described in the section on stability-sorting patterns. These procedures were used to conjecture that some of the conjectures of Graffiti were false, [12], conjecture 648, and they may be used in the construction of conceptual counterexamples, as mentioned in section 4.

It is nevertheless worth adding that the first question I am usually asked by students being introduced to the Red Burton style, is why the program will not find counterexamples to false conjectures on its own. Clearly, because otherwise students would have to start with proving theorems before acquiring intuitions and understanding of the problem, and primarily, because working on counterexamples is more fun, and because it is more educational. Nevertheless, students were of course right that by using very straightforward techniques like testing conjectures against lists of graphs or simple backtracking one could easily construct counterexamples to many, probably most, conjectures of Little Red Riding Hood.

Actually, to test the correctness of students' answers, I have a program which searches for the simplest counterexample. In its very first run the program found a simpler graph than the one claimed to be the simplest counterexample to the seventh round of the run discussed in section 12. Beforehand, the solver's solution (and the argument concerning simplicity, which even though incomplete,) seemed very reasonable to me, particularly that she was one of the best solvers of Little Red Riding Hood problems. The student was a computer science major who never took

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[12] On the basis of the performance of Glider, I conjecture that for every n, there is a $R(3,n)$-critical graph, which for every k less than n, contains a $R(3,k)$-critical graph. *Glider* provided only some experimental evidence that for every n there is a critical Ramsey graph $R(3,n)$ that can be extended to a critical Ramsey graph $R(3,n+1)$. Nevertheless, occasionally, I muster enough courage to make the strongest conjecture to which I do not know a counterexample – which is one of the guiding principles of the Dalmatian version.

any graph theory courses before and worked on these problems without academic credit, just for the fun of it.

Constructing smallest (forget simplest, which calls for a competent and thoughtful definition) counterexamples to conjectures of Red Burton may be a task easier for computers than for humans.[13] It is a part of Red Burton style, not because problems of this kind are necessarily easier, but because it is a kind of theorem-proving task about which even beginners do not have to ask, "Do I have a proof yet?" I am also often asked whether one could incorporate known results into Graffiti. It is a trivial task if the result is of the form which could be conjectured by Graffiti, which is of course true for many results in graph theory.

It is easy otherwise also, and I sometimes do it to speed up the computation of invariants by incorporating proved conjectures of Graffiti or known facts into the program. The structure of the program naturally provides facilities for doing this, but again it appears that so far there has not been much need for using them. Sometimes they may even be counterproductive, and they certainly are contrary to the principal idea and the spirit of the current versions of Graffiti, i.e., constructing hypothetical theories of its own. Graffiti for example never conjectured the nontrivial part of Brooks' Theorem, but it made the conjecture that the chromatic number of every graph G is not more than $1 + d_2$, where d_2 is the second largest term of the degree sequence of G. Brooks' theorem was an example of a result fed into Graffiti to speed up computation of the chromatic number, but leading Graffiti to the "discovery" of Brooks' bound would be pointless and might prevent the program from the discovery of the above bound.

15. Another example. We will finish with an example of a run of Little Red Riding Hood with essentially the same invariants as in section 12, but with the domain consisting of graphs of the form PR[n] discussed in sections 1, 4 and 9. Vertices of these graphs are numbers $2..n$, two being adjacent if and only if they are not relatively prime. The leading invariant is again the independence number which happens to be for these graphs $\pi(n)$ - the number of primes less or equal to n. Apart from being of interest for its own sake, this version is also an example of the program where in practise, the difficulties with the search for counterexamples are completely eliminated from the process, at least until the values of n will become prohibitively large.

There are other appealing aspects of this model which leads to various problems arising from full automation of Graffiti in the domain of Peano Arithmetic. In principle this very specific situation is general enough to study all of mathematics. The halting problem discussed at the end of section 8, becomes in this new setting the problem of finding a formula for $\pi(n)$ (depending on a set of initial invariants and a method of generating candidate conjectures).

Another interesting question is the decision problem whether the number of rounds in a run of Little Red Riding Hood for PR[n] graphs will be finite or infinite in those cases when the program will run forever. The same problems may be

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[13] This, of course, may very much depend on the domain of conjectures, but in the next section we discuss a version of Little Red Riding Hood where finding counterexamples does not present any difficulties in practice.

of equal interest for Gaussian integers, n-dimensional lattices and other countable domains starting with rationals, which, apart from obvious reasons, are of interest because the Tenth Hilbert Problem is still open for this field.

One of the first conjectures of this primality version of the program was that

$$\pi(n) \geq n - \Delta - 1$$

where Δ is the maximum degree of the graph $PR(n)$. The conjecture is of course false, yet it is difficult to overlook that it contains a hint directly leading to Euclid's proof of infinitude of primes. Indeed, if the number of primes were finite then their product (which would be a vertex of maximum degree) would dominate the graph for all sufficiently large n, which is a contradiction, because no vertex of PR[n] is adjacent to its successor nor the predecessor. In a nutshell, if the number of primes were finite then the conjecture would be true for large enough n.

References

[1] Philip Ball, Made to Measure, Princeton University Press 1997.

[2] Brigham and Dutton, INGRID, A Graph Invariant Manipulator, J. Symbolic Computation (1989) 7, 163 - 177.

[3] T. L. Brewster, M.J. Dinneen and V. Faber, Computational Attack on Conjectures of Graffiti: New Counterexamples and Proofs, Discrete Mathematics, 147, 1-3, (1995).

[4] F. Browder, Mathematical developments arising from Hilbert Problems, AMS 1976.

[5] Barbara Chervenka, Graffiti.pc Red Burton Style - A Student's Perspective, preprint, (2002).

[6] Noam Chomsky, Language and Thought, Anshen Transdisciplinary Lectures in Arts, Science and Philosophy of Culture, Moyer Bell (1993).

[7] Fan Chung, The Average Distance is not more than the Independence Number, Journal of Graph Theory, 12, 229-235, (1988).

[8] D.Cvetkovic, M.Doob and H.Sachs, Spectra of Graphs - Theory and Applications, 3rd revised and enlarged edition, Johann Ambrosius Barth Verlag, Heidelberg-Leipzig, 416 -417, (1995).

[9] Ermelinda DeLaVina, Graffiti.pc (pdf), Graph Theory Notes of New York Academy of Sciences, XLII, 26-30, (2002).

[10] Ermelinda DeLaVina, Graffiti.pc: A Variant of Graffiti, preprint, (2002).

[11] Siemion Fajtlowicz, Fullerene Expanders, a list of Conjectures of Minuteman, available from the author.

[12] Siemion Fajtlowicz, Written on the Wall, a list of Conjectures of Graffiti, available from the author.

[13] Siemion Fajtlowicz, Toward Fully Automated Fragments of Graph Theory, Graph Theory Notes of New York Academy of Sciences, XLII, 18-25, (2002).

[14] Siemion Fajtlowicz, Postscript to Fully Automated Fragments of Graph Theory, preprint 2002.

[15] Siemion Fajtlowicz, Examples are Forever, available from the author's webpage.

[16] Siemion Fajtlowicz, On Conjectures of Graffiti V, Proceedings of 7th International Quadrennial Conference on Graph Theory, Combinatorics and Applications, Western Michigan University '95, p. 367- 376.

[17] Siemion Fajtlowicz, On Conjectures and Methods of Graffiti, 4th Proceedings of Clemson Miniconference, (1989).

[18] Siemion Fajtlowicz, A proof of Inequality of Marcus and Lopes Algebra Universalis, 11 (1980), p. 264-266.

[19] Odile Favaron, M. Mahéo and J-F. Saclé, On the Residue of a Graph, Journal of Graph Theory, 15, 39-64, (1991).

[20] Patrick Fowler, Fullerene Graphs With More Negative Than Positive Eigenvalues; The Exceptions That Prove The Rule of Electron Deficiency, Journal Chem. Soc.Faraday, 93, 1-3, (1997).

[21] P. W. Fowler and D. E. Manolopoulos, An Atlas of Fullerenes, International Series of Monographs on Chemistry, 30, 1995.

[22] P. Fowler, K. Rodgers, S. Fajtlowicz, P. Hansen and G. Caporossi, Facts and Conjectures about Fullerene graphs, Leapfrog, Cylinder and Ramanujan Fullerenes, EuroConference Alcoma99, Springer May 2000, 134 - 146.

[23] Jerrold R. Griggs, Lower bounds on the independence number in terms of the degrees. J. Combin. Theory Ser. B 34 (1983) 22-39 05C15 (05C35)

[24] Jerrold R. Griggs and D.J. Kleitman, Independence and the Havel-Hakimi Residue, Discrete Mathematics, 127, 209-212, (1994).

[25] Frank Jelen, k-Independence and the k-residue of a graph, Journal of Graph Theory, 32, 241-249, (1999).

[26] Craig Larson, Intelligent Machinery and Mathematical Discovery, Graph Theory Notes of New York Academy of Sciences, XLII, 26-30, (2002).

[27] Craig Larson, An Updated Survey of Research in Automated Mathematical Conjecture-Making, preprint 2002.

[28] P. Langley, H. A. Simon, G. L. Bradshaw, and J. Zytkow, Scientific Discovery, The MIT Press, '1987.

[29] V. W. Marek and Jan Mycielski, Foundation of Mathematics in Twenthiest Century, http://spot.colorado.edu/ jmyciel/

[30] Fred Maxwell, Case Study: Graffiti Inspired Proof, classroom essay, 2001.

[31] Roger Penrose, Shadows of the Mind, Oxford University Press, 1994.

[32] Roger Penrose, The Large, the Small and the Human Mind, Cambridge University Press, 1997.

[33] Ryan Pepper, On New Didactics of Mathematics-Learning Graph Theory via Graffiti, preprint, (2002).

[34] Hillary Putnam, Mathematics Witout Foundations, Mathematics, Matter and Method, Cambridge University Press, 1975.

[35] Hillary Putnam, What is Mathematical Truth, Mathematics, Matter and Method, Cambridge University Press, 1975.

[36] Hillary Putnam, The Best of All Possible Brains?, The New York Times Book Review, Nov.20,1994, p.7.

[37] G. Ritchie and F. Hanna, AM: A Case Study in AI Methodology, Artificial Intelligence 23(3), 1984, 340-268.

[38] T. G. Schmalz, W. A. Seitz, D. J. Klein, and G. E. Hite, Proceedings of the 18th Conference on Carbon, Worcester, MA, (1987), p. 272 - 273.

[39] E. Triesch, Degree Sequences of Graphs and Dominance Order, Journal of Graph Theory, 22, 89-93, (1996).

[40] Hao Wang, Toward Mechanical Mathematics, in: Classical Papers on Computational Logic, 1957 - 1966, J. Siekmann and G. Wrifghtson, eds, Spriger-Verlag, 1983, 244-264.

[41] Joseph Weizenbaum, Computer Power and Human Reason, From Judgement to Calculation, W. H. Freeman and Company, 1976.

Nov. 30, 2002

[42] Pierre Hansen, How Far Should, Is AND Could Be Conjecture-Making Automated in Graph Theory, Les Cahiers du GERAD, G-2002-44, August 2002.

[43] Pierre Hansen, A. Aouchiche, G. Caporossi, D. Stevanovic, What Forms Do Interesting Conjectures Have in Graph Theory, Les Cahiers du GERAD, G-2002-46, August 2002.

[44] Siemion Fajtlowicz, Postscript to Fully Automated Fragments of Graph Theory, preprint 2002

[45] Siemion Fajtlowicz and Craig Larson, Graph-Theoretical Independence as a Predictor of Stability of Fullerenes, Chemical Physics Letters, 377 (2003) 485 - 490..

[46] Siemion Fajtlowicz, Hypotheses Concerning Stability of Fullerenes, CD ROM Proceedings of NASA NanoSpace 2001 Conference.

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