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Variable Neighborhood Search for Extremal Graphs 9. Bounding the Irregularity of a Graph

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ABSTRACT. Albertson [**1**] defines the *imbalance* of an edge $(i, j) \in E$ of a graph $G = (V, E)$ as $|d_i - d_j|$ where d_j is the degree of a vertex $j \in V$, and the *irregularity* $\mathrm{irr}(G)$ of G as the sum of imbalances of its edges. Exploiting conjectures of the system *AutoGraphiX*, an upper bound on $\mathrm{irr}(G)$ is derived, which is tight for all numbers $n = |V|$ and $m = |E|$ of vertices and edges compatible with the existence of a graph :

$$\mathrm{irr}(G) \leq d(n-d)(n-d+1) + t(t-2d-1)$$

where

$$d = \lfloor n - \frac{1}{2} - \sqrt{(n-\frac{1}{2})^2 - 2m} \rfloor$$

and

$$t = m - (n-d)d - d(d-1)/2.$$

Extremal graphs are shown to be *fanned split graphs*, i.e., complete split graphs with the possible addition of edges all incident with the same vertex.

1. Introduction

Let $G = (V, E)$ denote a simple, loopless, undirected graph with vertex set V and edge set E; let further $n = |V|$ and $m = |E|$ denote G's number of vertices and edges, and d_j, $j = 1, 2, \ldots, n$ the *degree* of (or number of edges incident with) vertex $j \in V$. If all d_j are equal G is *regular*. Otherwise G is *irregular*; however, it is of interest to measure how irregular it is. Several measures (which do not always agree) have been proposed for that purpose : Collatz and Sinogowitz [**10**] suggest to use the difference between the spectral radius λ_1 of the adjacency matrix and average degree $\frac{2m}{n}$ (they conjectured that stars maximize this difference, which was refuted by Cvetković and Rowlinson [**11**] using the system *GRAPH*); Bell [**3**] contrasts this measure with the variance of the degree sequence; Albertson [**1**] recently defined the *imbalance* of edge (i, j) as

$$\mathrm{imb}_{ij} = |d_i - d_j|$$

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i.e., the difference of the degrees of that edge's end vertices, in absolute value, and the *irregularity* $\mathrm{irr}(G)$ of a graph G as the sum of all edges imbalances :

$$\mathrm{irr}(G) = \sum_{(i,j)\in E} \mathrm{imb}_{ij} = \sum_{(i,j)\in E} |d_i - d_j|.$$

Note that all three measures are equal to zero for regular graphs. Tight upper bounds on the first two, expressed as functions of n and m for both connected and disconnected graphs are provided in [**3**] together with families of graphs for which these bounds are attained. It is shown in [**1**] that

$$\mathrm{irr}(G) < \frac{4n^3}{27},$$

and that this bound may be approached arbitrarily closely. However, no bound in function of n and m is given. It is the purpose of the present paper to fill in this gap by providing a formula which is best possible in the strong sense, i.e., which is tight for all values of n and m compatible with the existence of a graph. Moreover, extremal graphs are characterized and belong to a single well-defined family of split graphs.

These results were obtained using the system *AutoGraphiX* (*AGX*) [**8**] [**9**] for computed-assisted or (fully) automated graph theory. The aims of *AGX* are the following :

(1) Find graphs satisfying given constraints;
(2) Find graphs with optimal or near-optimal value of some invariant subject to constraints;
(3) Refute a conjecture;
(4) Find (or suggest) a new conjecture (or sharpen an existing one);
(5) Suggest a proof strategy.

These aims are attained by generating a large number of extremal or near-extremal graphs, using the Variable Neighborhood Search metaheuristic [**15**] [**16**]; then algebraic and / or structural conjectures are obtained interactively or automatically. Further details on *AGX*, and the three ways it uses to derive conjectures automatically are given in [**8**] [**9**]. Applications to graph theory are presented in these papers as well as in [**2**] [**5**] [**12**]. Moreover *AGX* is used to find and to help prove conjectures in chemical graph theory in [**4**] [**6**] [**13**] [**14**]. To find ideas of proof, the program is run with severe restrictions on the moves allowed within the heuristic (e.g. only rotation, or displacement, of a single edge at a time). If such moves suffice for obtaining again the extremal graphs previously found, the effort can be focused on proving that they suffice in general.

The paper is organized as follows : first experiments with *AGX* and their results, in terms of extremal graphs and 4 conjectures automatically obtained are described in the next section. They lead to conjecture a characterization of the family of extremal graphs and an upper bound on $\mathrm{irr}(G)$ in terms of n and m, presented in Section 3. Proofs of these conjectures are given in Section 4. A brief discussion concludes the paper in Section 5.

2. Experiments and automated conjectures

A short routine for computing the value of $\mathrm{irr}(G)$ was first programmed and added to *AGX*. Then it was asked to find graphs with maximal irregularity for

$3 \leq n \leq 12$ and $n-1 \leq m \leq \frac{n(n-1)}{2}$, as well as diagrams of these graphs, curves of values for a given n, and whatever conjectures might follow automatically. To find extremal graphs, the descent routine of AGX was used with the following neighborhoods: move of an edge, rotation of an edge, split and insertion; and a number of neighborhoods $k_{max} = 10$ (see [**8**] for details). To find conjectures on extremal graphs, the invariants $\omega(G)$ (clique number, or maximum number of pairwise adjacent vertices), $\alpha(G)$ (independence number, or maximum number of pairwise non-adjacent vertices), $\chi(G)$ (chromatic number or minimum number of colors to be assigned to the vertices of G in order not to have two adjacent vertices of the same color), r (radius of G or minimum over all vertices of G of the maximum distance to another vertex of G), Δ (maximum degree), and a few others were computed.

Then the numerical method described in [**7**] [**9**] was applied to find automatically a basis of affine relations between these invariants, satisfied by all extremal (or near-extremal) graphs found.

A subset of the 230 graphs obtained is presented in Figure 1; the corresponding curves of irr(G) for $9 \leq n \leq 12$, are drawn in Figure 2. Moreover, AGX provided the following 4 conjectures, which we group for conciseness :

Conjectures 1 to 4. *If G is a graph with n vertices, m edges, clique number $\omega(G)$, independence number $\alpha(G)$, chromatic number $\chi(G)$, maximum degree Δ, radius r and maximum irregularity irr(G), then*

$$\omega(G) = \chi(G), \tag{2.1}$$

$$n = \Delta + 1, \tag{2.2}$$

$$r = 1, \tag{2.3}$$

$$\omega(G) + \alpha(G) = \Delta + 2. \tag{2.4}$$

3. Interpretation and new conjectures

From the basis of affine relations given in Conjectures (2.1) to (2.4) one derives :

$$\omega(G) + \alpha(G) = n + 1; \tag{3.1}$$

so G comprises a clique C with $\omega(G)$ vertices and an independent set I with $\alpha(G)$ vertices which have a vertex in common. This implies they are specific *split graphs.* Indeed split graphs consist of a clique on n_1 vertices, a disjoint independent set on $n_2 = n - n_1$ vertices and possibly some edges joining a vertex of one set to one of the other. If all such edges are present G is a *complete split graph.* Replacing n by $n_1 + n_2$ in (3.1) and as $\alpha = n_2$ by definition of a split graph,

$$\omega(G) = n_1 + 1.$$

In other words, one vertex of the independent set is adjacent to all vertices of the clique in the split graph.

Moreover, one vertex at least is joined to all others, as $\Delta = n - 1$; this last relation implies $r = 1$ and conversely. Finally, the structure described implies $\chi(G) = \omega(G)$ as $\chi(G) \geq \omega(G)$ and a coloring in $\omega(G)$ colors can be obtained by giving the same color to all of the n_2 vertices of I and a different color to each remaining vertex.

This gives fairly good information on the structure of extremal graphs. However, a glance at these graphs themselves (see again Figure 1), and particularly at

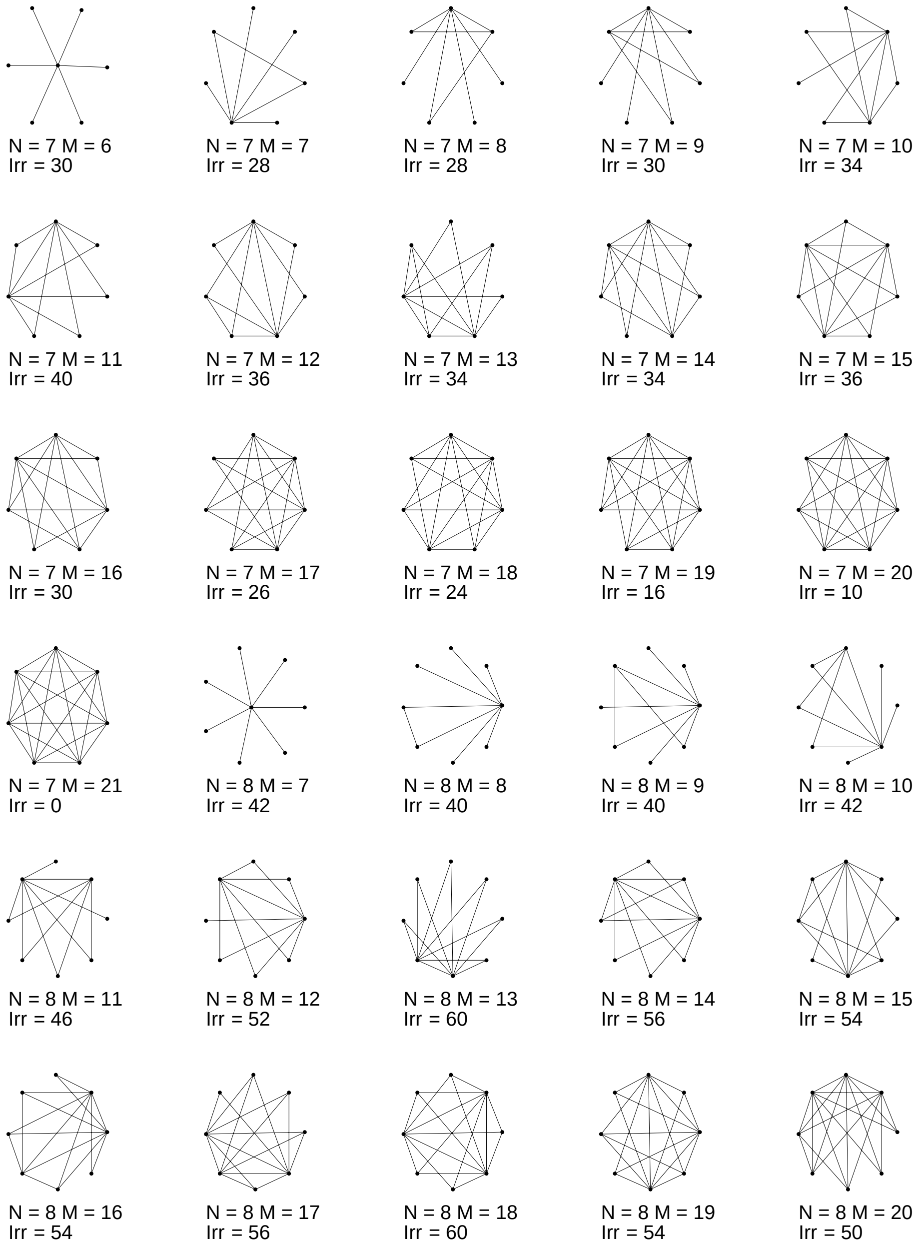

FIGURE 1. Some extremal graphs found by *AGX*

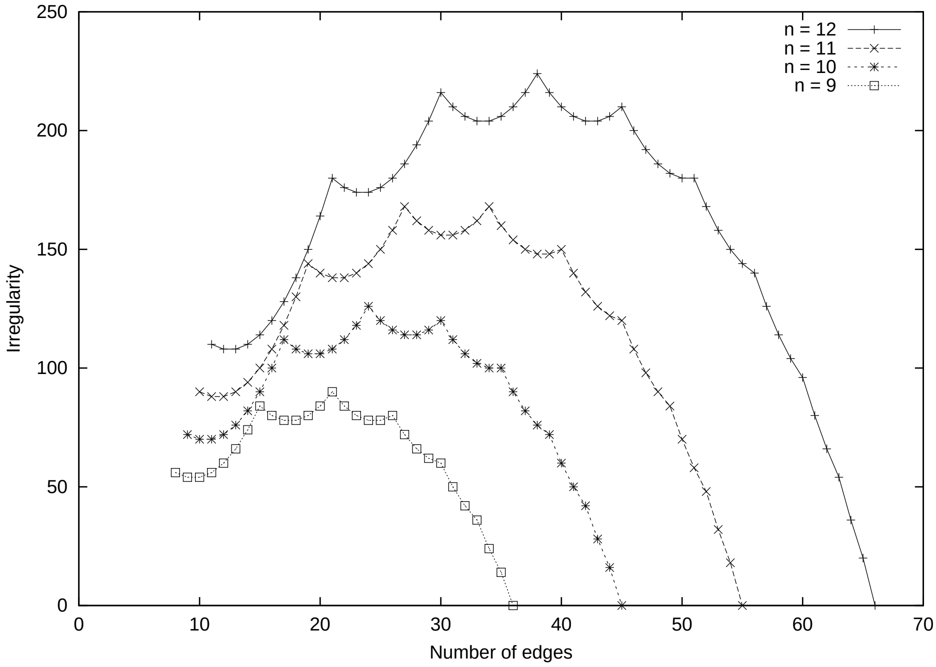

FIGURE 2. Values of Irregularity for some extremal graphs found by *AGX*

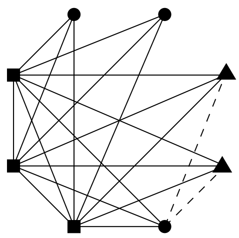

FIGURE 3. An example of fanned split graph with $n = 8$, $m = 20$, $d = 3$ (■) and $t = 2$ (▲)

successive ones with the same n and increasing m, shows one can say more. Indeed, they appear to be complete split graphs with a clique of d vertices, an independent set of $n - d$ vertices and possibly $1 \leq t \leq n - d - 1$ additional edges joining a vertex of the (previously) independent set to others of this set. We call such graphs *fanned split graphs* (as the addition of successive edges at a vertex is reminiscent of opening a fan). An example of a fanned split graph is presented in Figure 3 where $n = 8$, $m = 20$, $d = 3$ and $t = 2$. The three vertices of the clique are the black squares, and the dotted lines are the edges added from a vertex not in the clique to two other ones noted by triangles. So we can formulate the next conjecture (which is computer-aided, not automated, but for which the largest part of the job was clearly done by computer) :

Conjecture 5. *A graph G with n vertices and m edges has maximum irregularity if and only if it is a fanned split graph.*

A fanned split graph has

d vertices of degree $n-1$;
1 vertex of degree $d+t$;
t vertices of degree $d+1$;
$n-d-t-1$ vertices of degree d.

Moreover, G has $\frac{d(d-1)}{2}$ edges joining pairs of vertices of the clique, with imbalance 0; d edges joining vertices of the clique to the (first, if $t=1$) vertex of degree $d+t$, with imbalance $n-d-t-1$; dt edges joining vertices of the clique to vertices of degree $d+1$, with imbalance $n-d-2$; $d(n-d-t-1)$ edges joining a vertex of the clique to a vertex of degree d, with imbalance $n-d-1$; and t edges joining a vertex of degree $d+t$ to a vertex of degree $d+1$ with imbalance $t-1$.

Summing, one obtains for a fanned split graph $G = FS_{dt}$ an irregularity of

$$\mathrm{irr}(FS_{dt}) = d(n-d-t-1) + dt(n-d-2) + d(n-d-1)(n-d-t-1) + t(t-1).$$

A few algebraic manipulations then lead to

$$\mathrm{irr}(FS_{dt}) = d(n-d)(n-d-1) + t(t-2d-1). \tag{3.2}$$

So, if $t=0$ one gets the irregularity of a complete split graph with a clique on d vertices and an independent set on $n-d$ vertices, i.e., $d(n-d)(n-d-1)$. The effect of the additional t edges will reduce $\mathrm{irr}(G)$ if $t < 2d+1$, let it unchanged if $t = 2d+1$ and increase it if $t > 2d+1$. As shown on Figure 2, the local maxima for irregularity are obtained for complete split graphs.

From the definition of fanned split graph, one may easily compute d and t : indeed summing edges in the clique and between the clique and the independent set gives that d is the largest integer such that

$$\frac{d(d-1)}{2} + d(n-d) \le m$$

from where it follows that

$$d = \lfloor n - \frac{1}{2} - \sqrt{(n-\frac{1}{2})^2 - 2m} \rfloor \tag{3.3}$$

where $\lfloor b \rfloor$ denotes the largest integer not larger than b and

$$t = m - (n-d)d - d(d-1)/2. \tag{3.4}$$

Note that these graphs are unique for fixed numbers n of vertices and m of edges.

We summarize these results in the following conjecture :

Conjecture 6. *For all graphs G with n vertices and m edges the irregularity*

$$\mathrm{irr}(G) \le d(n-d)(n-d-1) + t(t-2d-1) \tag{3.5}$$

where d and t are given by (3.3) and (3.4). Moreover, the bound is attained for all n and $0 \le m \le \frac{n(n-1)}{2}$.

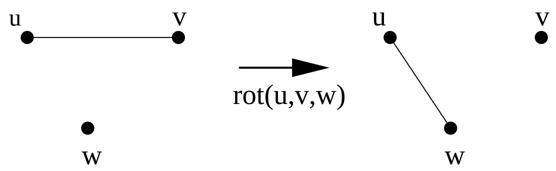

FIGURE 4. A rotation $\mathrm{rot}(u, v, w)$

4. Proofs

Before looking for a proof of the conjectures, we ran AGX with only one move allowed within the heuristic : we chose the simplest one for which the number of vertices and edges are not altered, i.e., rotation of a single edge. Let G be a graph and u, v, w three different vertices of G such that $(u, v) \in E(G)$ and $(u, w) \notin E(G)$; one can define the graph G' obtained after rotation $\mathrm{rot}(u, v, w)$ is applied to G as follows :

$$G' = G - (u, v) + (u, w).$$

Such a move is represented in Figure 4.

With this restriction, AGX found again systematically the fanned split graphs as extremal graphs. This observation led us to use the graphical interface of AGX, which permits to modify the graphs manually and see how the invariants change in consequence. Such manipulation, together with the information on the structure of the fanned split graph collected before, led us to write the following algorithm which transform any graph G with n vertices and m edges into a fanned split graph with the same number of vertices and edges, using only rotation.

FANNEDSPLITGRAPH(G):
Input: a graph G with n vertices and m edges.
Output: a fanned split graph with the same numbers of vertices and edges.

(1) *Initialization.*
   (a) Let F be the set of vertices of G with a degree equal to $n - 1$. We call them the *fixed* vertices in the next steps.
   (b) *Stop* $\leftarrow FALSE$.
   (c) *Choose* w. Choose a non-fixed vertex w with maximum degree.
(2) *Make a move.* While *Stop* is $FALSE$, do
   (a) *Choose* u. Choose a non-fixed vertex $u \neq w$, not adjacent to w.
      (i) If $d_u > |F|$, choose any non-fixed vertex v such that $(u, v) \in E(G)$ and do $\mathrm{rot}(u, v, w)$.
      (ii) Else ($d_u = |F|$), try to find an edge (v_1, v_2) where $\{v_1, v_2\} \notin F \cup w$ and $d_{v_1} \geq d_{v_2}$.
         (A) If such an edge exists, do $\mathrm{rot}(v_1, v_2, u)$ followed by $\mathrm{rot}(u, v_1, w)$.
         (B) If not, *Stop* $\leftarrow TRUE$.
   (b) *Update* F. If $d_w = n - 1$, $F = F \cup w$ and choose a new w as a non-fixed vertex of maximum degree.

LEMMA 4.1. *Algorithm **FannedSplitGraph** terminates if and only if G has been transformed into a fanned split graph.*

PROOF. Let $x_1, x_2, \ldots x_f$ be the fixed vertices of G (with degree equal to $n-1$). Let w be the vertex of maximum degree $< n-1$. We see that in step **2**, a move will always increase the degree of w. Indeed this algorithm will stop only if we can no more add an edge to w, i.e. if $f = d$ and if there is no more edge (v_1, v_2) between vertices of the set $V(G) \setminus F \setminus w$. This situation occurs only when G is a fanned split graph with the value d and t defined above.

Note that if $m < n-1$ this algorithm will construct a graph composed of a star with $m+1$ vertices and $n-m-1$ isolated vertices which is a fanned split graph also. Moreover if G is not connected and if $m \geq n-1$, this algorithm will choose w as the vertex of maximum degree until $d_w = n-1$. At this step G will be (and remain) connected.

Remark also that u, a vertex non-adjacent to w, can always be chosen in step **2a** because $d_w < n-1$ (otherwise w would be fixed) and if $d_u > |F|$, a vertex v can always be found because u is adjacent to the f fixed vertices and has at least one another edge to a vertex $\neq w$. $\square$

We can now verify what AGX suggest to us. To do this, let us define some notations introduced by Albertson [**1**]. If $u \in V(G)$,

$$d_u^> = |\{x : (x,u) \in E(G) \text{ and } d_u > d_x\}|,$$

$$d_u^= = |\{x : (x,u) \in E(G) \text{ and } d_u = d_x\}|,$$

and

$$d_u^< = |\{x : (x,u) \in E(G) \text{ and } d_u < d_x\}|.$$

Remark that $d_u = d_u^> + d_u^= + d_u^<$.

LEMMA 4.2 (Edge Rotation Lemma). *Let u, v, w be three different vertices of G. If $(u,v) \in E(G)$ and $(u,w) \notin E(G)$, set $G' = G - (u,v) + (u,w)$. Then we have the following results:*

If $d_u \geq d_v$ and $d_u > d_w$	$irr(G') = irr(G) + 2[d_v^< + d_v^= - d_w^< - 1] + k$	*Case 1*
If $d_u \geq d_v$ and $d_u \leq d_w$	$irr(G') = irr(G) + 2[d_v^< + d_v^= + d_w^> + d_w^= - d_u] + k$	*Case 2*
If $d_u < d_v$ and $d_u > d_w$	$irr(G') = irr(G) + 2[d_u - d_v^> - d_w^<] + k$	*Case 3*
If $d_u < d_v$ and $d_u \leq d_w$	$irr(G') = irr(G) + 2[d_w^> + d_w^= - d_v^> + 1] + k$	*Case 4*

where $k = 2$ if $(v,w) \in E(G)$ and $d_v = d_w + 1$, and $k = 0$ otherwise.

PROOF. Suppose first that there is no edge between v and w. The imbalance of the edges of G' will change only on the edges adjacent with the vertices v and w in G. We will compute the contribution of the moving edge $(u,v) \to (u,w)$, of the edges adjacent with w in G and of the edges adjacent to v in G different from (u,v).

- The contribution of the moving edge will be

$$|d_u - (d_w + 1)| - |d_u - d_v|. \tag{4.1}$$

- The total contribution of the edges adjacent with w in G will be

$$d_w^> + d_w^= - d_w^<. \tag{4.2}$$

- Finally, the contribution of the edges adjacent with v different from (u,v) will be

$$d_v^< + d_v^= - d_v^> - 1 \quad \text{if} \quad d_u \geq d_v \tag{4.3}$$

$$d_v^< + d_v^= - d_v^> + 1 \quad \text{if} \quad d_u < d_v \tag{4.4}$$

because the moving edge, for which the imbalance has already been computed, counts for one in $d_v^< + d_v^=$ if $d_u \geq d_v$ or in $d_v^>$ otherwise.

Summing these contributions leads to the four cases (with $k = 0$) and where we compare d_u and d_w also to remove the absolute value in expression (4.1).

Suppose now that there exist an edge (v, w). The contributions will be similar of the previous one but we count the edge (v, w) twice : once in (4.2) and once in (4.3) or (4.4). In fact, the contribution of this edge will be

$$|(d_v - 1) - (d_w + 1)|. \tag{4.5}$$

Depending of d_v and d_w, this leads to several cases where we look how this edge was counted twice, the contribution already counted in the previous sum, and the value of imb_{vw} induced by (4.5) :

Assumption	Counted in	previous count	imb_{vw}
$d_v > d_w + 1$	$d_v^>$ and $d_w^<$	-2	-2
$d_v = d_w + 1$	$d_v^>$ and $d_w^<$	-2	0
$d_v = d_w$	$d_v^=$ and $d_w^=$	2	2
$d_v < d_w$	$d_v^<$ and $d_w^>$	2	2

There is only a difference when $d_v = d_w + 1$, which justifies the values of k in Lemma 4.2. □

Lemma 4.3. *Running the **FannedSplitGraph** algorithm on any graph G which is not a fanned split graph will strictly increase irregularity.*

Proof. If G is a fanned split graph, the algorithm will not do any move. Otherwise, there will be at least one move. So we only have to prove that steps **2(a)i** and **2(a)ii** will strictly increase irregularity of G.

Let $f = |F|$ be the number of vertices of degree $n - 1$. As in steps **1c** or **2b** w is chosen such as d_w is maximum among the non-fixed vertices :

$$d_w^< = f; \tag{4.6}$$

$$d_y^< \geq f; \tag{4.7}$$

$$d_y^> + d_y^= + d_y^< \leq d_w^> + d_w^= + d_w^<; \tag{4.8}$$

for any non-fixed vertex y. Expressions (4.6) and (4.7) give

$$d_w^< \leq d_y^< \tag{4.9}$$

and, subtracting in both sides of (4.8)

$$d_y^> + d_y^= \leq d_w^> + d_w^=. \tag{4.10}$$

Let u be the vertex chosen in step **2a**.

- Suppose first that $d_u > f$. In this case, a vertex v is selected in step **2(a)i** and rotation $\mathrm{rot}(u, v, w)$ applied on G.

  By the choice of w and u, it is easy to check that $d_u < d_w$, and we have two cases :
  - If $d_u < d_v$, we are in Case 4 of Lemma 4.2 ,

    $$\mathrm{irr}(G') = \mathrm{irr}(G) + 2[d_w^> + d_w^= - d_v^> + 1] + k,$$

    and as v is non-fixed (4.10) implies that $\mathrm{irr}(G') > \mathrm{irr}(G)$.

– If $d_u \geq d_v$, we are in Case 2 :

$$\operatorname{irr}(G') = \operatorname{irr}(G) + 2[d_v^< + d_v^= + d_w^> + d_w^= - d_u] + k,$$

and as $d_u < d_w$,

$$d_v^< + d_v^= + d_w^> + d_w^= - d_u > d_v^< + d_v^= + d_w^> + d_w^= - d_w = d_v^< + d_v^= - d_w^<$$

which is positive as $d_v^< \geq d_w^<$ by (4.9). Again, $\operatorname{irr}(G') > \operatorname{irr}(G)$.

- Suppose now that $d_u = f$. In this case, one tries to find an edge (v_1, v_2) in step **2(a)ii** such that $\{v_1, v_2\} \notin F \cup w$ and $d_{v_1} \geq d_{v_2}$. Then two rotations are applied on G. Let G' be the graph obtained after rotation $\operatorname{rot}(v_1, v_2, u)$ is applied on G and G'' the graph obtained after rotation $\operatorname{rot}(u, v_1, w)$ is applied on G'. As some degrees will change after the first rotation, we will note them d_i' in G'. By construction $d_{v_1} \geq d_{v_2} > d_u = f$ which means that we are in Case 1 of Lemma 4.2 for the first rotation :

$$\operatorname{irr}(G') = \operatorname{irr}(G) + 2[d_{v_2}^< + d_{v_2}^= - d_u^< - 1] + k$$

where $k = 0$ because there is no edge (v_2, u) and where $d_u^< = d_u = f$. So,

$$\operatorname{irr}(G') = \operatorname{irr}(G) + 2[d_{v_2}^< + d_{v_2}^= - f - 1]. \tag{4.11}$$

Let us see now how the degrees have changed before the second rotation. It is clear that

$$d_u' = d_u + 1, d_{v_1}' = d_{v_1} \text{ and } d_w' = d_w \tag{4.12}$$

but some other changes can happen in the decomposition of these degrees in the sets $d^<, d^>$ and $d^=$. There are three different possible configurations :

(1) $d_{v_1} > d_{v_2}$. As $d_{v_2} \geq d_u + 1$ and by (4.12) we have $d_{v_1}' > d_u'$. Moreover, $d_w' \geq d_u'$ and we are in Case 4 of Lemma 4.2:

$$\operatorname{irr}(G'') = \operatorname{irr}(G') + 2[d_w^{>'} + d_w^{='} - d_{v_1}^{>'} + 1] + k$$

where $k \geq 0$ and where $d_{v_1}^{>'} = d_{v_1}^>, d_w^{>'} = d_w^>$ and $d_w^{='} = d_w^=$. Finally, replacing $\operatorname{irr}(G')$ by (4.11) gives

$$\operatorname{irr}(G'') = \operatorname{irr}(G) + 2[d_{v_2}^< + d_{v_2}^= - f - 1 + d_w^> + d_w^= - d_{v_1}^> + 1] + k.$$

which is strictly greater than zero because $d_{v_2}^< \geq f + 1$ (the f edges from v_2 to the fixed vertices, plus the edge (v_1, v_2)) and $d_w^> + d_w^= \geq d_{v_1}^>$ by (4.10).

(2) $d_{v_1} = d_{v_2}$ and $d_{v_2} > d_u + 1$. We are again in Case 4 but the difference here is that $d_{v_1}^{>'} = d_{v_1}^> + 1$:

$$\operatorname{irr}(G'') = \operatorname{irr}(G) + 2[d_{v_2}^< + d_{v_2}^= - f - 1 + d_w^> + d_w^= - d_{v_1}^>] + k.$$

which is strictly greater than zero because $d_{v_2}^< \geq f + 1$, $d_w^> + d_w^= \geq d_{v_1}^>$ as before and $d_{v_2}^= \geq 1$ due to the edge (v_1, v_2).

(3) $d_{v_1} = d_{v_2}$ and $d_{v_2} = d_u + 1$. In this last case, $d_{v_1}' = d_u'$ and $d_w' \geq d_u'$, so we are in Case 2 :

$$\operatorname{irr}(G'') = \operatorname{irr}(G') + 2[d_{v_1}^{<'} + d_{v_1}^{='} + d_w^{>'} + d_w^{='} - d_u'] + k.$$

One can check that $k = 0$, $d'_u = f + 1$, $d^{='}_{v_1} = 1$, $d^{<'}_{v_1} = f$, $d^{>'}_w = d^>_w$ and $d^{='}_w = d^=_w$. Putting these values in the previous expression and replacing irr(G') by (4.11) leads to

$$\mathrm{irr}(G'') = \mathrm{irr}(G) + 2[d^<_{v_2} + d^=_{v_2} + d^>_w + d^=_w - f - 1],$$

which is strictly positive because $d^=_{v_2} = 1$, $d^{<'}_{v_2} = f$ and $d^>_w > 0$.

□

THEOREM 4.4. *(Conjectures 5 and 6) For any graph G with n vertices, m edges and irregularity irr(G),*

$$irr(G) \leq d(n-d)(n-d+1) + t(t-2d-1)$$

where

$$d = \lfloor n - \frac{1}{2} - \sqrt{(n-\frac{1}{2})^2 - 2m} \rfloor$$

and

$$t = m - (n-d)d - d(d-1)/2.$$

Moreover, this value is attained if and only if G is a fanned split graph.

PROOF. From Lemma 4.1, algorithm **FannedSplitGraph** applied to any graph G ends with the unique fanned split graph with n vertices and m edges. From Lemma 4.3 all rotations or pairs of rotations applied increase strictly the irregularity of the graph. It follows that fanned split graphs are extremal (which is Conjecture 5). Then the bound follows from the computations preceeding Conjecture 6. The fact that it is best possible and that extremal graphs can be characterized as fanned split graphs follows also from Lemmas 4.1 and 4.3. □

5. Concluding remarks

The problem of finding a best possible bound on the irregularity of graphs G with n vertices and m edges, as defined by Albertson [**1**], is entirely solved. Moreover, extremal graphs are characterized.

These results could be obtained through three of the main capacities of the system *AutoGraphiX* [**8**] [**9**] :

(1) Finding extremal or near extremal graphs. In this case *AGX* obtained 230 graphs which were extremal, without one exception.
(2) Finding automatically conjectures. Four such conjectures were obtained, from which it follows that extremal graphs are split graphs with one vertex of largest possible degree.

    Using these results and the representation of graphs found, a new family of graphs was identified : *fanned split graphs*, which are complete split graphs with possibly some additional edges all incident with a same vertex. The 230 graphs obtained all belong to this family, which has one and only one member for each pair of numbers n of vertices and m of edges compatible with existence of a graph. The conjectures that extremal graphs always belong to this family, as well as a numerical bound on irregularity, follow.

(3) Suggesting proof strategies. The extremal graphs obtained could be found once again using only the edge rotation move, which is the simplest one leaving n and m unchanged. This suggested an algorithm to go from any graph G to a fanned split graph with the same number of vertices and edges, using only moves which increase irregularity. Such an algorithm using one or two rotations at each step could be obtained, with help of the interactive component of AGX. The two conjectures were thus proved.

We believe the "simulated algorithm" type of proof used here to be worthy of further study.

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