LINEAR INEQUALITIES AMONG GRAPH INVARIANTS: USING GRAPHEDRON TO UNCOVER OPTIMAL RELATIONSHIPS

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Abstract. Optimality of a linear inequality in finitely many graph invariants is defined through a geometric approach. For a fixed number of graph nodes, consider all the tuples of values taken by the invariants on a selected class of graphs. Then form the polytope which is the convex hull of all these tuples. By definition, the optimal linear inequalities correspond to the facets of this polytope. They are finite in number, are logically independent, and generate precisely all the linear inequalities valid on the class of graphs. The computer system GraPHedron, developed by some of the authors, is able to produce experimental data about such inequalities for a “small” number of nodes. It greatly helps conjecturing optimal linear inequalities, which are then hopefully proved for any node number. Two examples are investigated here for the class of connected graphs. First, all the optimal linear inequalities in the stability number and the link number are obtained. To this aim, a problem of Ore (1962) related to Turán Theorem (1941) is solved. Second, several optimal inequalities are established for three invariants: the maximum degree, the irregularity, and the diameter.

Key words. graph invariants, polytope, optimal linear inequalities, GraPHedron

AMS subject classifications. 05C35, 52B12, 90C35

1. Introduction. An important research stream in Graph Theory studies relationships among graph invariants. Invariants are numerical indices which summarize the graph structure: their values are preserved by isomorphisms. Relations among invariants range from very easy (such as: the sum of node degrees equals twice the number of links) to very deep and difficult (like many results in extremal graph theory). During the last two decades, several computer based systems have been developed in order to generate new relations among invariants. Some of them even produced conjectures in an automated way; see [34] for a survey emphasizing contributions to algebraic graph theory. Here is a brief sketch of the main existing systems (among others):

• the GRAPH system by Cvetković et al. [16, 17, 18, 19, 20, 21] allows interactive computing of invariants and includes also a theorem-proving component;
• the INGRID system of Brigham and Dutton [6, 7, 8, 9] implements manipulation of formulae involving graph invariants;
• the Graffiti system of Fajtlowicz et al. [23, 24, 25, 26, 27, 28, 29] generates a priori conjectures and then eliminates those that are rejected by a database of counter-examples or are not interesting;
• the AutoGraphiX system of Caporossi and Hansen [2, 10, 11, 12, 13, 22, 30, 33] generates extremal or near-extremal graphs for some relations on graph invariants, then derives conjectures along different methods.

Hansen [31] divides such computer systems into two classes: automated systems which provide conjectures in a fully automated way (i.e., without human intervention.

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apart for the problem statement), and computer-assisted systems otherwise. The new system we have implemented is a computer-assisted one.

The investigation of relations among graph invariants should tackle the following two general questions: when is a relation interesting? when is it optimal? Here, we derive answers to the latter questions from a polyhedral approach. The approach is quite natural, so we suppose that it was applied before the writing of this paper. We just mention that Caporossi and Hansen [13] also view graphs as points in a space of invariants, although they explore only a selection of graphs which are extremal or near-extremal for a given objective function. As explained below, our approach allows to single out a finite number of optimal relations from which all other relations follow.

Given a fixed set of $p$ invariants for graphs, linear inequalities among these invariants are of a particular interest. According to our general point of view, we consider all linear inequalities which hold for graphs from a given class $C$ (e.g., the class of connected graphs with $n$ nodes*). Each graph $G$ from the class $C$ is represented by some point in the $p$-dimensional real space $\mathbb{R}^p$: the point has its coordinates equal to the values taken by the $p$ invariants for $G$. The convex hull of all the resulting points (obtained when $G$ varies in $C$) is the polytope of graph invariants for the selected set of invariants and the class $C$ of graphs. Any linear inequality on $\mathbb{R}^p$ valid for the polytope of graph invariants induces a linear relationship among the invariants under investigation, which holds for the class $C$. Furthermore, such an inequality can be considered as best possible exactly when it defines a facet of the polytope. The reason is twosome: all other linear inequalities among the invariants are logical consequences (even, are dominated by a positive combination) of the facet defining inequalities, and no facet defining inequality can be a logical consequence of other such inequalities. Besides, these facet defining inequalities are finite in number; we will refer to them as the optimal inequalities. Notice also that a description by optimal inequalities of the polytope of graph invariants can be of great help when a linear combination of the invariants has to be maximized over the graphs in the class $C$. We remark in passing that the above approach also applies to nonlinear relationships among invariants: it suffices to associate coordinates to, say, powers or products of invariants.

The polyhedral interpretation of the linear inequalities among the $p$ selected graph invariants also suggests a fruitful strategy to formulate conjectures. The first three stages can be implemented on a computer. First, for $n$ not too large, generate all the graphs on $n$ nodes which belong to the class $C$ under study (the program geng [37] can be instrumental, maybe supplemented with ad hoc routines). Second, compute for each graph the values taken by the graph invariants. Third, for any $n$ in the admissible range, determine in $\mathbb{R}^p$ the convex hull of the resulting $p$-dimensional points (running for instance the software porta [14]). Fourth, interpret the facet defining inequalities which were obtained for the various values of $n$. The strategy helps conjecturing linear inequalities among the selected invariants. There remains to mathematically establish these relationships in full generality for the class $C$. Two applications of the strategy are provided in this paper.

The method can be used to verify whether known inequalities among invariants are best possible in a very strong sense. To the contrary, it is a common practice to show that a given inequality among invariants is tight by exhibiting an instance for which the relation holds with equality. This argument shows only that the inequality defines a supporting hyperplane of the convex hull defined above. It does not establish

*For the sake of clarity, we reserve the terms 'vertices' and 'edges' for convex polytopes, and thus speak of 'nodes' and 'links' of graphs.
Optimal linear inequalities

that the inequality defines a facet. This last property, according to our approach, singles out the optimal linear inequalities.

In the next section, we provide a brief description of the computer system designed to support our investigations (see Mélot [38] for technical details). The system heavily relies on the programs geng [37] and porta [14]. In order to perform exact arithmetic, it treats only invariants taking rational values. One of its distinctive features is the automatic production of a report summarizing information on the polytope of graph invariants, such as the list of vertices, the list of facets, drawings of graphs (just one, or all) which produce any given vertex, etc.

Apart from a brief section containing general definitions, the rest of the paper illustrates our approach with results obtained in two cases for the class of connected graphs. First, we limit ourselves to a case of two invariants, namely the stability number and the link number. Our system produced figures of the resulting polytope for the number of graph nodes raising up to 11. We were then able to establish the complete list of facet defining inequalities for all values of $n$. On the way, we solve a problem raised by Ore [39] in relation with Turán Theorem (thus improving recent results of Harant and Schiermeyer [36]). The problem asks for the least number of links in a connected graph on $n$ nodes with $m$ links and stability number $\alpha$. Turán [40] solved the similar problem for general graphs by describing nonconnected optimal solutions.

A second illustration is a case with three invariants, the maximum degree, the diameter and the irregularity. Several optimal linear inequalities are obtained. However, determining the complete list of all such inequalities remains an open problem.

2. Outline of the system GraPHedron. The main steps in using the system GraPHedron are as follows.

Problem statement. The system GraPHedron is able to handle (undirected, simple) graphs. However, the graphs can be restricted to belong to some special class, e.g., by requiring the graph to be connected, biconnected, triangle-free, 4-cycle-free, bipartite, a tree, a chemical graph, ... Routines for selecting all graphs in a special class, or directly generating them, are included in or can be added to the system. For instance, the program geng [37] is incorporated as a subroutine. Besides the graph class, the user also selects some invariants $i_1, i_2, \ldots, i_p$, e.g., number of links, diameter, maximum degree, ... New invariants can be easily added to the system.

Data generation. All the nonisomorphic graphs for a given class and a given number of nodes $n$ are generated and stored in a compressed format for future use. As we are limited by CPU time and storage capacity, we can only generate the graphs for "small" values of $n$. Table 2.1 records (estimations of) the resources needed in the case of connected graphs (for which the limitation today is $n = 11$). These results were obtained on a Linux computer with a Pentium (R) IV (3 GHz) processor. Of course, for more restricted classes, the manageable number $n$ of nodes can reach larger values. For example, Table 2.2 refers to the class of trees.

For each selected invariant, its value for all the graphs generated is computed and stored. Again, this computation will be made only once. This is very useful when computing the invariant takes a long time. Every graph has its own reference which allows for a direct access to the graph and its (previously computed) invariants.

Determination of optimal linear inequalities between invariants. For each $n$, the system determines all the different coordinate vectors and keeps a reference to the graphs corresponding to every such vector (the number of graph references stored can be lim-
Table 2.1

<table>
<thead>
<tr>
<th>$n$</th>
<th># of graphs generated</th>
<th>CPU time</th>
<th>File size</th>
</tr>
</thead>
<tbody>
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<td>21</td>
<td>0.00 sec</td>
<td>0.144 Kb</td>
</tr>
<tr>
<td>6</td>
<td>112</td>
<td>0.00 sec</td>
<td>0.321 Kb</td>
</tr>
<tr>
<td>7</td>
<td>853</td>
<td>0.01 sec</td>
<td>2.7 Kb</td>
</tr>
<tr>
<td>8</td>
<td>11 117</td>
<td>0.03 sec</td>
<td>44 Kb</td>
</tr>
<tr>
<td>9</td>
<td>261 080</td>
<td>0.45 sec</td>
<td>171 Kb</td>
</tr>
<tr>
<td>10</td>
<td>11 716 571</td>
<td>20.94 sec</td>
<td>6.96 $\times$ 10$^4$ Kb</td>
</tr>
<tr>
<td>11</td>
<td>1 006 700 565</td>
<td>29 min 29.66 sec</td>
<td>6.82 $\times$ 10$^6$ Kb</td>
</tr>
<tr>
<td>12</td>
<td>$1.64 \times 10^{11}$</td>
<td>(est.) 3.5 days</td>
<td>(comp.) 1.44 $\times$ 10$^9$ Kb</td>
</tr>
<tr>
<td>13</td>
<td>$5.03 \times 10^{13}$</td>
<td>(est.) 2.8 years</td>
<td>(comp.) 4.92 $\times$ 10$^{11}$ Kb</td>
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</table>

Table 2.2

<table>
<thead>
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<th># of graphs generated</th>
<th>CPU time</th>
<th>File size</th>
</tr>
</thead>
<tbody>
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<td>3</td>
<td>0.00 sec</td>
<td>0.109 Kb</td>
</tr>
<tr>
<td>10</td>
<td>106</td>
<td>0.01 sec</td>
<td>0.725 Kb</td>
</tr>
<tr>
<td>15</td>
<td>7 741</td>
<td>1.28 sec</td>
<td>105.94 Kb</td>
</tr>
<tr>
<td>20</td>
<td>823 065</td>
<td>11 min 58.93 sec</td>
<td>1.9 $\times$ 10$^4$ Kb</td>
</tr>
<tr>
<td>25</td>
<td>104 636 890</td>
<td>(est.) 7.5 days</td>
<td>(comp.) 3.88 $\times$ 10$^6$ Kb</td>
</tr>
</tbody>
</table>

3. Notations. Let $G = (V, E)$ be a connected graph with node set $V$ and link set $E$. As usual, the number of nodes of the graph $G$ is denoted by $n = |V|$ and the number of links by $m = |E|$. A set $A$ of nodes of $G$ is stable if $\{v, w\} \notin E$ for all $v, w \in A$. The maximum cardinality of a stable set of $G$ is the stability number $\alpha(G)$. We denote by $d_v$ the degree of node $v$, that is $d_v = |\{w \in V : \{v, w\} \in E\}|$, and by $\Delta(G)$ the maximum degree, thus $\max_{v \in V} d_v$. The distance between two nodes $v$ and $w$ is the length of a shortest path from $v$ to $w$. The diameter $D(G)$ is the maximum distance between two nodes of $G$. A diameter path in $G$ is a path of length $D(G)$. The irregularity of $G$ is $\iota(G) = \sum_{(v, w) \in E} |d_v - d_w|$.

Let us quickly provide a motivation for the last parameter. A graph $G$ is regular if all the degrees of its nodes are equal, otherwise $G$ is irregular. Clearly, it is of interest to measure how much $G$ is irregular. Among the measures of irregularity proposed in the literature, the most prevalent ones are: the Collatz-Sinogowitz index which is the difference between the largest eigenvalue of the adjacency matrix and the average degree [15]; the variance of degrees [3] and, more recently, the irregularity of

Edited). This set of coordinate vectors is sent to porta [14], which then finds the facets and the vertices of the convex hull and outputs the optimal inequalities (which are in bijection with the facets) and the vertex coordinates.

Interactive visualization of the results and derivation of conjectures. The user has to study the inequalities by hand or by interacting with the system to see and/or print the graphs corresponding to a certain vertex. In the case of two invariants, the automatic report produced by the system contains a drawing of the polygon of graph invariants. For three invariants, it will be possible in the future to visualize and manipulate the three dimensional polyhedron.
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Albertson [1], which we use here. Note that all these indices are equal to zero if $G$ is regular.

A star is a tree with one node adjacent to all other nodes. Other classical graphs will also be used, such as the complete graph $K_n$, the complete bipartite graph $K_{a,b}$, the path $L_n$, the cycle $C_n$. Additional graphs are introduced when needed.

A polytope is the convex hull $\text{conv} S$ of a finite set $S$ of points in $\mathbb{R}^d$. For terminology about polytopes, we generally follow Ziegler [41].

4. Stability Number and Link Number. The general methodology outlined in the Introduction is applied here to the case of two invariants, the stability number and the link number. Fixing the number $n$ of nodes, we associate to any connected graph $G = (V, E)$ on $n$ nodes the pair $(\alpha, m)$ where, as before, $\alpha = \alpha(G)$ and $m = |E|$. Our goal is to determine, for any $n$, all facet defining inequalities for the convex polygon

$$P_{\alpha,m}^n = \text{conv} \{ (\alpha, m) : \text{there exists a connected graph } G = (V, E) \text{ with } |V| = n, \alpha(G) = \alpha, |E| = m \}.$$  

The polygon $P_{\alpha,m}^n$ lies in a plane $\mathbb{R}^2$ having two coordinates $x_\alpha$ and $x_m$. For $n = 10$, it is illustrated in Figure 4.1.

Figure 4.1, together with similar figures for other values of $n$, suggests to sort out the edges of $P_{\alpha,m}^n$ in three families. These families respectively consist of: (i) one horizontal edge lying on the line $x_m = n - 1$; (ii) edges to the right, forming a path from vertex $(n - 1, n - 1)$ to vertex $(1, \binom{n}{2})$; (iii) edges to the left, connecting vertex $(\lfloor \frac{n+1}{2} \rfloor, n - 1)$ to vertex $(1, \binom{n}{2})$. Our analysis will treat these three families one after the other, and establish in each case the complete list of edges together with the corresponding facet defining inequalities. To avoid trivialities, we will assume $n \geq 4$ in this section.

4.1. The horizontal edge. Since we consider only connected graphs on $n$ nodes, the minimum number of links in such a graph equals $n - 1$, a value which arises exactly for trees. The stability number of such trees varies from $\lfloor \frac{n+1}{2} \rfloor$ (for a path on $n$ nodes) to $n - 1$ (for a star $K_{1,n-1}$). There results a horizontal edge for $P_{\alpha,m}^n$, with vertices $(\lfloor \frac{n+1}{2} \rfloor, n - 1)$ and $(n - 1, n - 1)$. The corresponding facet defining inequality is of course $x_m \geq n - 1$.

4.2. The rightmost edges. The following proposition handles the second family of edges.

**Proposition 4.1.** For $k = 1, 2, \ldots, n - 2$, the inequality

$$kx_\alpha + x_m \leq \binom{n-k}{2} + kn$$  

(4.2)

defines an edge of $P_{\alpha,m}^n$ with vertices

$$\left(k, \binom{n-k}{2} + k(n-k)\right) \text{ and } \left(k + 1, \binom{n-k}{2} + k(n-k - 1)\right).$$  

(4.3)

All edges and vertices of $P_{\alpha,m}^n$ to the right of some point of $P_{\alpha,m}^n$ are of these types.

There results the sequence of vertices $\left(k, \binom{n-k}{2} + k(n-k)\right)$ for $k = 1, 2, \ldots, n - 1$, which starts at $(1, \binom{n}{2})$ and ends at $(n - 1, n - 1)$. Two successive vertices in
the sequence have their abscissas differing by 1. Hence $P^n_{\alpha,m}$ has no other vertex on the rightmost part of its boundary.

**Proof.** We first establish that Inequality (4.2) is valid for each vertex of $P^n_{\alpha,m}$. With $\alpha$ denoting the stability number of a graph $G = (V, E)$ for which $|V| = n$ and $|E| = m$, this amounts to prove

$$m \leq \left( \frac{n-k}{2} \right) + k(n-\alpha).$$

(4.4)
We proceed by considering two cases.

a) Case $k \leq \alpha$. In some stable set $S$ of maximum size in $G$, select some subset $T$ of $k$ nodes. The number of links disjoint from $T$ is at most $\binom{n-k}{2}$. Any other link has exactly one node in $T$; its other node lies outside $S$. The number of such links is at most $k(n-\alpha)$. Summing up, we get Inequality (4.4).

b) Case $k > \alpha$. Select a set $U$ of $k$ nodes which contains a maximum-size stable set $S$. Any link is either (i) disjoint from $U$, or (ii) formed by one node in $S$ and the other one in $V \setminus S$, or (iii) formed by one node in $U \setminus S$ and the other one in $V \setminus S$. Thus the total number of links is at most $\binom{n-k}{2} + \alpha(n-\alpha) + (k-\alpha)(n-\alpha)$, from which Inequality (4.4) follows.

We thus have proved that Inequality (4.2) holds for $P_{n,\alpha,m}$.

Each of the two points given in (4.3) comes from at least one connected graph, namely the graph having as links all those pairs of nodes not included in a fixed subset of $k$, resp. $k+1$, nodes. As easily checked, these two points satisfy Inequality (4.2) with equality, and the same for a second linear inequality also valid for the polytope. Consequently, these two points are the vertices lying on the edge defined by Inequality (4.2). Moreover, there can be no other edge because we have found vertices with abscissas increasing by step of 1 from 1 to $n-1$.

We point out that another proof of Proposition 4.1 can be forged by first finding out vertices, which means: (i) determining the maximum number of links in a connected graph with given number of nodes and given stability number; (ii) showing that the resulting points in $\mathbb{R}^2$ are convexly independent. The easy solution to (i) states that the maximum number of links equals $(n-\alpha)(n+\alpha-1)/2$. As this function of $\alpha$ is strictly concave, (ii) becomes trivial. Inequality (4.2) can then be derived. This line of argument produces also a nonlinear inequality attributed to Tomescu in [32]:

$$\alpha \leq \left\lfloor \frac{1}{2} + \sqrt{\frac{1}{4} + n(n-1) - 2m} \right\rfloor$$

4.3. The leftmost edges. For the third and last family of edges, we will first infer the corresponding vertices from the answer to the following question: what is the minimum number of links in connected graphs with fixed number of nodes and fixed stability number? This question is listed as an open problem in Ore [39]. A complete answer is contained in Proposition 4.3 below. It constitutes the variant for connected graphs of a celebrated result of Turán [40], which we now recall. For given integer numbers $n$ and $\alpha$ satisfying $n \geq \alpha \geq 1$, the Turán graph $T(n,\alpha)$ has $n$ nodes and is the disjoint union of $\alpha$ cliques with balanced sizes (i.e., sizes equal to $\lfloor \frac{n}{\alpha} \rfloor$ or $\lceil \frac{n}{\alpha} \rceil$; the last two expressions give the same value if and only if $\alpha$ divides $n$). We let $t(n,\alpha)$ denote the number of links in the Turán graph $T(n,\alpha)$.

**Proposition 4.2.** [40]. Any graph on $n$ nodes with stability number $\alpha$ has at least $t(n,\alpha)$ links. Moreover, this graph has exactly $t(n,\alpha)$ links iff it is (isomorphic to) the Turán graph $T(n,\alpha)$.

Thus the only graph with minimum number of links in Proposition 4.2 has $\alpha$ connected components. Of course, by adding $\alpha-1$ carefully selected links, we obtain various connected graphs on $n$ nodes and stability number $\alpha$. Notice that in case $n = 2\alpha + 1$, odd cycles on $n$ nodes still provide other examples with the same values of $\alpha$ and $m$. Despite their diversity, we are able to prove that all these connected graphs have the minimum possible number of links for given $n$ and $\alpha$. The proof is more involved than the simple ones known for Turán result (and exposed e.g. in...
Bollobás [5]). Also, it covers more cases than the connected one (which is obtained in Proposition 4.3 below for \( c = 1 \), see Corollary 4.7).

**Proposition 4.3.** Any graph \( G \) on \( n \) nodes with stability number \( \alpha \) and with \( c \) connected components has at least \( t(n, \alpha) + \alpha - c \) links. The lower bound is tight in all cases.

For \( 1 \leq c \leq \alpha \leq n \), let \( f_c(n, \alpha) \) be the minimum number of links for graphs as in Proposition 4.3. To prove \( f_c(n, \alpha) = t(n, \alpha) + \alpha - c \), we first establish two lemmas (a third one comes later).

**Lemma 4.4.** Suppose \( n \geq 2 \alpha \). If \( f_1(n, \alpha) = t(n, \alpha) + \alpha - 1 \), then for \( c = 1, 2, \ldots, \alpha \), we have \( f_c(n, \alpha) = t(n, \alpha) + \alpha - c \).

**Proof.** (of Lemma 4.4) The assumption \( n \geq 2 \alpha \) implies that each maximal clique of the Turán graph \( T(n, \alpha) \) has more than one node. By adding \( \alpha - c \) carefully selected links to \( T(n, \alpha) \), we see

\[
 t(n, \alpha) + \alpha - c \geq f_c(n, \alpha),
\]

and similarly by adding \( c - 1 \) carefully selected links to a graph realizing \( f_c(n, \alpha) \),

\[
 f_c(n, \alpha) + c - 1 \geq f_1(n, \alpha).
\]

Thus

\[
 t(n, \alpha) + \alpha - c \geq f_c(n, \alpha) \geq f_1(n, \alpha) - (c - 1).
\]

By our assumption, the first and last expressions in Equation (4.5) are equal. The thesis follows. \( \square \)

**Lemma 4.5.** For \( 1 \leq \beta \leq \alpha \leq n \), we have

\[
 t(n, \beta) \geq t(n, \alpha) + \alpha - \beta.
\]

**Proof.** (of Lemma 4.5) We need consider only the case \( \alpha = \beta + 1 \). To transform \( T(n, \beta + 1) \) into \( T(n, \beta) \), we pick a clique of size \( \left\lfloor \frac{n}{\beta + 1} \right\rfloor \) in the first graph, delete its nodes and add \( \left\lfloor \frac{n}{\beta + 1} \right\rfloor \) nodes in all to the other cliques. Clearly, the number of links increases at each deletion/addition of a single node. \( \square \)

**Proof.** (of Proposition 4.3) By Lemma 4.4, we need to establish the thesis only for \( G \) connected. We prove \( f_1(n, \alpha) = t(n, \alpha) + \alpha - 1 \) by recurrence on the number \( n \) of nodes. Remark that inequality \( f_1(n, \alpha) \leq t(n, \alpha) + \alpha - 1 \) holds in view of the connected graphs mentioned before Proposition 4.3, which are built by adding \( \alpha - 1 \) well-chosen links to the Turán graph \( T(n, \alpha) \). Hence, there only remains to prove the following inequality:

\[
 f_1(n, \alpha) \geq t(n, \alpha) + \alpha - 1.
\]

Assume first \( n \leq 2 \alpha \). Then \( t(n, \alpha) = n - \alpha \) because the Turán graph then consists of \( 2 \alpha - n \) isolated nodes plus \( n - \alpha \) parallel edges. On the other hand, any connected graph on \( n \) nodes has at least \( n - 1 \) links, thus \( f_1(n, \alpha) \geq n - 1 = t(n, \alpha) + \alpha - 1 \), which gives Inequality (4.7).

Assume now \( n > 2 \alpha \). Let \( S \) be a maximum stable set of \( G \), and let \( b \) be the number of connected components of \( G \setminus S \) (thus \( b \leq \alpha \)).

By Lemma 4.6 below, the number of links in the cut \( \delta(S) \) is at least \( n - \alpha + b - 1 \). On the other hand, \( G \) induces on \( V \setminus S \) a graph with \( b \) components and stability
number \( \beta \) satisfying \( \beta \leq \alpha < n - \alpha \). By the induction assumption together with Lemma 4.4, the graph induced on \( V \setminus S \) has at least \( f_b(n - \alpha, \beta) = t(n - \alpha, \beta) + \beta - b \) links. Summing up, we get

\[
m \geq n - \alpha + b - 1 + t(n - \alpha, \beta) + \beta - b
\]

and then by Lemma 4.5

\[
m \geq n - \alpha + b - 1 + t(n - \alpha, \alpha) + \alpha - \beta - b
\]

\[
= n - \alpha + t(n - \alpha, \alpha) + \alpha - 1
\]

\[
= t(n, \alpha) + \alpha - 1
\]

(the last equality directly derives from the structure of Turán graphs: the adjunction of a vertex to each of the \( \alpha \) maximal cliques of \( T(n - \alpha, \alpha) \) produces \( T(n, \alpha) \)). Inequality (4.7) is now proved in all cases.

The last assertion in Proposition (4.3) is correct in view of the examples provided just before the statement. \( \mathbb{D} \)

**Lemma 4.6.** As in the proof of Proposition 4.3, let \( G = (V, E) \) be a connected graph with \( n \) nodes, \( m \) links and stability number \( \alpha \). Take a maximum stable set \( S \) in \( G \), and let \( C_1, C_2, \ldots, C_b \) be the \( b \) connected components of \( G \setminus S \). Then

\[
|\delta(S)| \geq n - \alpha + b - 1.
\]  

(4.8)

**Proof.** (of Lemma 4.6) For \( i = 1, 2, \ldots, b \), build a spanning tree of \( C_i \). Then extend the union of these \( b \) (sub)trees into a spanning tree \( T \) of \( G \). Clearly, \( E(T) \cap \delta(S) \) is an acyclic set of links of \( G \) which covers \( S \) and at least one node in each \( C_i \) (maybe several nodes in a given \( C_i \)). Denote by \( G' \) the graph \( (V, E(T) \cap \delta(S)) \) and let \( A_1, A_2, \ldots, A_\ell \) be the connected components with more than one node of \( G' \). For \( j = 1, 2, \ldots, \ell \), denote by \( s_j \) (resp. \( r_j \)) the number of nodes of \( A_j \) in \( S \) (resp. not in \( S \)). Thus, the subgraph of \( G' \) induced by \( A_j \) is a tree with \( s_j + r_j \) nodes (see Figure 4.2 for an illustration).

![Fig. 4.2. An example of graph G for the proof of Lemma 4.6. The links in E(T) are shown in bold lines.](image)

For any fixed \( j \), two nodes in \( A_j \setminus S \) cannot belong to the same \( C_i \) (otherwise there would be a cycle formed by links of the tree \( T \)). We derive

\[
\sum_{j=1}^{\ell} (r_j - 1) = b - 1
\]

(4.9)
by repeatedly collapsing nodes as follows. Say $A_j$ and $A_j'$ have each a node in a same $C_i$. Then by collapsing these two nodes we collect $A_j$ and $A_j'$, together while leaving the left-hand side of Equation (4.9) unchanged because $(r_j - 1) + (r_j' - 1) = (r_j + r_j' - 1) - 1$. All such collapsings done, there remains in the left-hand side of Equation (4.9) only one term which equals $b - 1$ because exactly one node remains in each of the $b$ sets $C_i$'s.

We now establish a lower bound on the number $p_j$ of links of $G$ connecting the $r_j$ nodes in $A_j \setminus S$ to (whatever) nodes of $S$. By connectivity of $A_j$, we surely have $p_j \geq s_j + r_j - 1$.

**First case:** $s_j \geq r_j$. Then we get $p_j \geq 2r_j - 1$.

**Second case:** $s_j + 1 \leq r_j$. We prove $p_j \geq 2r_j - 1$ here also, by finding additional links. Let

$$A_j \setminus S = \{v_1, v_2, \ldots, v_{r_j}\},$$

$$A_j \cap S = W \quad \text{(thus } |W| = s_j \text{)}.$$  

As $(S \setminus W) \cup \{v_1, v_2, \ldots, v_{s_j+1}\}$ contains $\alpha + 1$ nodes, it cannot be a stable set of $G$. As both $S \setminus W$ and $\{v_1, v_2, \ldots, v_{r_j}\}$ are stable (the latter because as shown before $A_j \setminus S$ cannot have two nodes in a same $C_i$), there must be a link connecting $S \setminus W$ to some node in $\{v_1, v_2, \ldots, v_{s_j+1}\}$, say $v_1$. This link differs from the $s_j + r_j - 1$ links found before. The same argument when $v_1$ is replaced with $v_{s_j+2}$ will produce a new link from, say, $v_2$ to $S \setminus W$. Repeating again the argument with $v_{s_j+3}, v_{s_j+4}, \ldots, v_{r_j}$ taken into account, we get $(s_j + r_j - 1) + (r_j - s_j)$ links connecting $A_j \setminus S$ to $S$, and thus $p_j \geq 2r_j - 1$.

Consider now any node $u$ of $G$ not covered by $E(T) \cap \delta(S)$, thus $u \not\in S$. As $S \cup \{u\}$ cannot be stable, there is some link connecting $u$ to $S$.

Finally, any node outside $S$ is either covered by $E(T) \cap \delta(S)$ (and then, for some $j$, belongs to $A_j$) or is not covered (and then is adjacent to some vertex in $S$). Using also $p_j \geq 2r_j - 1$ and Equation (4.9), we get

$$|\delta(S)| \geq \left( \sum_{j=1}^\ell (2r_j - 1) \right) + \left( n - \alpha - \sum_{j=1}^\ell r_j \right)$$

$$= n - \alpha + \sum_{j=1}^\ell (r_j - 1)$$

$$= n - \alpha + b - 1.$$  

The most important case in Proposition 4.3 comes when $c = 1$. In view of the following explicit form of the Turán number (see e.g. [4])

$$t(n, \alpha) = \left( \left\lceil \frac{n}{\alpha} \right\rceil - 1 \right) \cdot \left( n - \alpha \left\lceil \frac{n}{\alpha} \right\rceil \right),$$

(4.10)

we thus have proved the next result.

**Corollary 4.7.** The minimum number of links for all connected graphs on $n$ nodes with stability number $\alpha$ equals

$$\left( \left\lceil \frac{n}{\alpha} \right\rceil - 1 \right) \cdot \left( n - \alpha \left\lceil \frac{n}{\alpha} \right\rceil \right) + \alpha - 1.$$  

(4.11)
Optimal linear inequalities

Corollary 4.7 improves the main result in [36], which consists in a lower bound on the minimum number of links.

We now determine the leftmost vertices and edges of the polytope $P^m_{a,m}$, taking advantage of the following points of $P^m_{a,m}$ delivered by Corollary 4.7:

\[ p_k = (k, t(n, k) + k - 1), \quad \text{for } k = 1, 2, \ldots, \left\lceil \frac{n+1}{2} \right\rceil. \]  

(4.12)

A first step is to show that all of these points are boundary points. Next, we determine which of them are vertices. The edges then follow at once (see Corollary 4.9).

**Proposition 4.8.** The vertices of the leftmost part of the boundary of $P^m_{a,m}$ are exactly the points provided in Equation (4.12) for $k$ in \(\{2, 3, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor\} \) satisfying

\[ \left\lfloor \frac{n}{k-1} \right\rfloor \neq \left\lceil \frac{n}{k+1} \right\rceil + 1, \]  

(4.13)

and also for $k = 1$ and $k = \left\lfloor \frac{n+1}{2} \right\rfloor$.

**Proof.** Leaving aside the vertices $(1, \binom{n}{2})$ and $(\left\lfloor \frac{n+1}{2} \right\rfloor, n - 1)$, we assume $1 < k < \left\lfloor \frac{n+1}{2} \right\rfloor$ in the rest of the proof. To establish that the point $p_k$ is on the boundary of $P^m_{a,m}$, it suffices to show that the “Turán function” (for a fixed value of $n$)

\[ t(n, x) : \left\{1, 2, \ldots, \left\lfloor \frac{n+1}{2} \right\rfloor\right\} \to \mathbb{R} : x \mapsto t(n, x) \]  

(4.14)

is the restriction of a convex function from $[1, \left\lfloor \frac{n+1}{2} \right\rfloor]$ to $\mathbb{R}$ (notice that we may discard the affine term $k - 1$ which appears in the second coordinate of $p_k$, because it does not alter convexity). In turn, we need only prove for $k = 2, 3, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor$

\[ t(n, k) \leq \frac{1}{2} \left(t(n, k - 1) + t(n, k + 1)\right). \]  

(4.15)

Inequality (4.15) follows from the following three assertions (again for $k = 2, 3, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor$): The line with equation

\[ x_m - t(n, k) = -\left(\left\lceil \frac{n}{k} \right\rceil + 1\right) (x_\alpha - k) \]  

(4.16)

1. goes through the point $p_k = (k, t(n, k))$,
2. supports the point $p_{k-1} = (k-1, t(n, k - 1))$, and
3. supports the point $p_{k+1} = (k+1, t(n, k + 1))$.

The first assertion is clear. Setting $s = \left\lfloor \frac{n}{k} \right\rfloor$, we see that the second one is equivalent to

\[ t(n, k - 1) - t(n, k) \geq \left(s + 1\right). \]  

(4.17)

We derive the latter inequality by checking how many new links are created when the Turán graph $T(n, k)$ is transformed into the similar graph $T(n, k - 1)$. As explained before Proposition 4.2, the graph $T(n, k)$ is a union of cliques with size equal to $s$ and maybe also $s + 1$. To transform it into $T(n, k - 1)$, we select a clique with size $s$ and
move its nodes one after the other to other cliques. At the first step, we lose \( s - 1 \) links in the clique to be deleted, and gain at least \( s \) links in the augmented clique; in all, we gain at least one link. For the second node, we have a gain of at least 2 (because we lose \( s - 2 \) links this time), etc. Thus the total number of links increases by at least \( 1 + 2 + \cdots + s \), that is \( \binom{s+1}{2} \).

Now the third assertion about the line in Equation (4.16) translates into

\[
t(n, k) - t(n, k + 1) \leq \binom{s+1}{2}.
\]

(4.18)

The graph \( T(n, k+1) \) is a union of \( k+1 \) cliques, of size say \( d \) and (maybe also) \( d+1 \). To transform \( T(n, k+1) \) into \( T(n, k) \), we move all nodes of some clique of size \( d \) to other cliques. As we can create cliques only of size \( s \) or \( s+1 \) (because of the structure of \( T(n, k) \)), the number of links increases by at most \( s - (d-1) \) at the first move, then at most \( s - (d-2) \), etc.; at the last move, we gain at most \( s \) links. Hence the increase in the number of links is bounded above by \( \frac{1}{d+1} (2s+1 - d) \). For \( s \) fixed, this quantity is maximized for \( d = s \) or \( d = s+1 \). We conclude that Assertion 3 is correct.

Having thus shown that all points \( p_k \) provided in (4.12) are on the boundary of \( P^m_{n, \alpha} \), we notice next that all leftmost vertices of \( P^m_{n, \alpha} \) must be among the \( p_k \)'s (because two successive points \( p_k \) have their abscissas differing by 1). Also, a point \( p_k \) is not a vertex if and only if the line in Equation (4.16) goes also through the points \( p_{k-1} \) and \( p_{k+1} \), which happens exactly if we have equality in both Inequalities (4.17) and (4.18). By inspecting the arguments which led to these inequalities, it is easily seen that both equalities occur if and only if the sizes of the maximal cliques in \( T(n, k-1) \), resp. \( T(n, k+1) \), are all also sizes of maximal cliques in \( T(n, k) \). This is equivalent to saying that \( n/(k+1) \) and \( n/(k-1) \) lie in an interval with endpoints equal to two consecutive integers. Finally, \( p_k \) is not a vertex if and only if \( \left\lceil \frac{n}{k-1} \right\rceil = \left\lfloor \frac{n}{k+1} \right\rfloor + 1 \).

Example. For \( n = 24 \), the values of \( k \) which do not provide a vertex are 7 and then 9, 10, 11. In particular, all points \( p_9, p_{10}, p_{11} \) lie on the segment joining the vertices \( p_8 \) and \( p_{12} \).

Corollary 4.9. The leftmost edges of \( P^m_{n, \alpha} \) are defined by the following inequalities:

\[
x_m - t(n, k) - (k-1) \geq (t(n, k) - t(n, k-1) + 1) (x_\alpha - k)
\]

(4.19)

for values \( k = 2, 3, \ldots, \left\lfloor \frac{n+1}{2} \right\rfloor \) satisfying \( \left\lfloor \frac{n}{k-1} \right\rfloor \neq \left\lfloor \frac{n}{k+1} \right\rfloor + 1 \).

We have completed our analysis of the case with the two invariants \( \alpha \) and \( m \). The full list of optimal linear inequalities appears in Table 4.1. The polygon \( P^m_{n, \alpha} \) has an interesting property which is not shared by all similar polytopes constructed for other choices of invariants: Any point from \( P^m_{n, \alpha} \) which has integer coordinates is produced by some graph in the class considered (here, the class of connected graphs on \( n \) nodes).

5. Maximum Degree, Irregularity and Diameter. Our methodology is now applied to the following three invariants of a connected graph \( G \) : the maximum degree \( \Delta(G) \), the irregularity \( \iota(G) \) and the diameter \( D(G) \). The polytope of graph invariants
### Table 4.1

<table>
<thead>
<tr>
<th>m</th>
<th>( \geq n - 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k \alpha + m )</td>
<td>( \leq \binom{n-k}{2} + kn ) for ( k = 1, 2, \ldots, n - 2 )</td>
</tr>
</tbody>
</table>
| \( m - t(n,k) - (k-1) \) | \( \geq \) for \( k = 2, 3, \ldots, \left\lceil \frac{n+1}{2} \right\rceil \) with \( \left\lfloor \frac{n}{k-1} \right\rfloor \neq \left\lfloor \frac{n}{k+1} \right\rfloor + 1 \)

is here

\[ P_{\Delta,\iota,D}^n = \text{conv}\{(\Delta, \iota, D) \in \mathbb{Z}^3 : \text{there exists a connected graph } G = (V,E) \text{ with } |V| = n, \Delta(G) = \Delta, \iota(G) = \iota \text{ and } D(G) = D\}. \quad (5.1) \]

For any fixed \( n \), the polytope \( P_{\Delta,\iota,D}^n \) lies in the 3-dimensional space \( \mathbb{R}^3 \) with coordinates \( x_\Delta, x_\iota \text{ and } x_D \). As shown in the next proposition, it is full-dimensional. Consequently, the facets of \( P_{\Delta,\iota,D}^n \) are its 2-dimensional faces.

**Proposition 5.1.** Let \( P_{\Delta,\iota,D}^n \) be the polytope defined by (5.1). If \( n \geq 4 \), then \( \dim(P_{\Delta,\iota,D}^n) = 3 \).

**Proof.** To exhibit four affinely independent points lying in \( P_{\Delta,\iota,D}^n \), consider the following graphs on \( n \) nodes: the complete graph \( K_n \), the cycle \( C_n \), the star \( K_{1,n-1} \), and the path \( L_n \). The corresponding points, namely

- \( K_n : (n-1,0,1) \),
- \( C_n : (2,0,\lfloor n/2 \rfloor) \),
- \( K_{1,n-1} : (n-1,(n-1)(n-2),2) \),
- \( L_n : (2,2,n-1) \).

They are easily seen to be affinely independent. \[ \square \]

The output produced by GraPhedron for \( n = 4, 5, \ldots, 10 \) led us to conjecture that (under various assumptions) five families of linear inequalities are facet defining. We proceed to give the corresponding proofs.

**Proposition 5.2.** If \( n \geq 4 \), the inequality

\[ x_\Delta \leq n - 1 \quad (5.2) \]

is facet defining for \( P_{\Delta,\iota,D}^n \).

**Proof.** The validity of Inequality (5.2) for \( P_{\Delta,\iota,D}^n \) is obvious. Because the origin does not belong to the affine plane \( \Pi \equiv x_\Delta = n - 1 \), it is now sufficient to exhibit three linearly independent vectors of \( P_{\Delta,\iota,D}^n \) belonging to \( \Pi \). Let us consider the following three graphs: the complete graph \( K_n \), the star \( K_{1,n-1} \), and finally \( G_3 \), a star augmented with one link. The corresponding vectors, namely

- \( K_n : (n-1,0,1) \),
- \( K_{1,n-1} : (n-1,(n-1)(n-2),2) \),
- \( G_3 : (n-1,n(n-3),2) \),
belong to \( H \cap P^n_{\Delta, r, D} \) and are linearly independent. \( \square \)

**Proposition 5.3.** The inequality
\[
x_\Delta + x_D \leq n + 1 \tag{5.3}
\]
is facet defining for \( P^n_{\Delta, r, D} \) when \( n \geq 4 \).

**Proof.** (i) We first prove that \( \Delta(G) + D(G) \leq n + 1 \) holds for any connected graph \( G \) on \( n \).
Take a diameter path \( P \) of \( G \), thus \( P \) is a shortest path \( v_1, v_2, \ldots, v_{D(G)+1} \) (with length \( D(G) \)). Let \( v^* \) be a node having degree \( \Delta(G) \) and \( N(v^*) \) be the neighborhood of \( v^* \), i.e. \( N(v^*) = \{ v \in V : \{ v, v^* \} \in E \} \cup \{ v^* \} \). From

\[
|P| + |N(v^*)| - |P \cap N(v^*)| \leq n,
\]

\[
|P| = D(G) + 1, \quad |N(v^*)| = \Delta(G) + 1,
\]
we derive

\[
\Delta(G) + D(G) + 2 - |P \cap N(v^*)| \leq n.
\]

It remains to prove \( |P \cap N(v^*)| \leq 3 \).

1. Suppose \( P \cap N(v^*) = \emptyset \). Then \( |P \cap N(v^*)| = 0 \leq 3 \).
2. Suppose \( P \cap N(v^*) \neq \emptyset \) and \( v^* \notin P \). Then \( |P \cap N(v^*)| \leq 3 \), otherwise \( P \) could not be a shortest path.
3. Suppose \( P \cap N(v^*) \neq \emptyset \) and \( v^* = v_k \in P \). If \( 1 < k < D(G) + 1 \), then
\[
P \cap N(v^*) = \{ v_{k-1}, v^*, v_{k+1} \}
\]
because \( P \) is a shortest path, and so \( |P \cap N(v^*)| = 3 \).
If \( v^* = v_1 \) or \( v^* = v_{D(G)+1} \), then \( |P \cap N(v^*)| = 2 \).

(ii) Having proved that Inequality (5.3) is valid for \( P^n_{\Delta, r, D} \), we now show that it defines a facet. The path \( L_n \), the star \( K^1_{1,n-1} \), and the star augmented with one link, denoted as \( G_3 \) in the proof of Proposition 5.2, produce the vectors

\[
(2, 2, n-1), \quad (n-1, (n-1)(n-2), 2), \quad (n-1, n(n-3), 2).
\]

These three vectors satisfy (5.3) with equality and, when \( n \geq 4 \), they are linearly independent. \( \square \)

Let \( H = (V(H), E(H)) \) be a subgraph of \( G = (V, E) \). We define the irregularity along \( H \) as
\[
\varepsilon(H) = \sum_{k \in E(U)} |d_k - d_l|
\]
where the degree \( d_k \) of node \( k \) is relative to the graph \( G \). To establish in Proposition 5.5 the validity of our next inequality, we first improve Inequality (5.3).

**Lemma 5.4.** Let \( G = (V, E) \) be a connected graph such that \( \varepsilon(G) < \Delta(G) \). Then
\[
\Delta(G) + D(G) \leq n.
\]

**Proof.** We show for any connected graph \( G \) that \( \Delta(G) + D(G) > n \) implies \( \varepsilon(G) \geq \Delta(G) \). By Inequality (5.3), we may assume \( \Delta(G) + D(G) = n + 1 \). From the proof of Proposition 5.3, any node of maximum degree must be on some diameter path. Let \( P = v_1, v_2, \ldots, v_{D(G)+1} \) be a diameter path containing at least one node of degree \( \Delta(G) \).

By construction, the diameter path \( P \) contains \( D(G) + 1 \) nodes. Consequently, \( n - (D(G) + 1) = \Delta(G) - 2 \) nodes do not belong to \( P \). We call them exterior nodes (relatively to diameter path \( P \)) and denote them by \( w_1, w_2, \ldots, w_{\Delta(G)-2} \). The extremities \( v_1 \) and \( v_{D(G)+1} \) of the diameter path \( P \) are of degree at most \( \Delta(G) - 1 \). So, let \( v^* = v_k \in P \setminus \{ v_1, v_{D(G)+1} \} \) be the node of \( P \) with maximum degree such that the subpath \( P_k \subset P \) which joins \( v_1 \) to \( v^* \) does not contain any other node of maximum degree. There are \( \Delta(G) \) links incident to the node \( v^* \) and two of them belong to the
Fig. 5.1. All the exterior nodes are adjacent to the node $v^*$. In Case (a), one has $d_{v_1} = 1$, while in Case (b), one has $1 < d_{v_1} \leq \Delta - 1$.

diameter path $P$. Thus the $\Delta(G) - 2$ remaining links are incident to the $\Delta(G) - 2$ exterior nodes. We consider two cases (see Figure 5.1).

Case (a). Suppose $d_{v_1} = 1$. By comparing the degrees along $P_1$, we obtain for the irregularity along $P_1$

$$\iota(P_1) \geq \Delta(G) - 1.$$ 

Case (b). Suppose now $d_{v_1} = d > 1$. (Note that the distance between $v_1$ and $v^*$ cannot be greater than two, in other terms: $v^* = v_2$ or $v^* = v_3$.) We have

$$\iota(P_1) \geq \Delta(G) - d.$$ 

All the nodes adjacent to $v_1$, but one, are exterior nodes. Let $P_2, P_3, \ldots, P_d$ be the paths defined by $P_r = \{v_1, w_{r-1}, v^*\}$ (after relabelling the exterior nodes if necessary). Because the paths $P_1, P_2, \ldots, P_d$ have no common link, there follows

$$\sum_{r=1}^{d} \iota(P_r) \geq d(\Delta(G) - d).$$

Moreover, $2 \leq d \leq \Delta(G) - 1$, which implies

$$d(\Delta(G) - d) \geq \Delta(G) - 1.$$ 

This proves

$$\sum_{r=1}^{d} \iota(P_r) \geq \Delta(G) - 1.$$ 

Now in both Cases (a) and (b) let $P_0$ be the subpath of $P$ joining $v^*$ to $v_{\Delta(G) + 1}$. Clearly, the irregularity along $P_0$ is at least 1, and so

$$\iota(G) \geq \Delta(G).$$
The inequality
\[ nx_\Delta - x_s + (n-1)x_D \leq n^2 - 1 \] (5.6)
is valid for \( P^{n}_{\Delta, \iota, D} \). If \( n \geq 5 \) and \( n \) is odd, the inequality is facet defining.

Proof. (i) We first prove the validity of Inequality (5.6). For a graph \( G = (V, E) \), this inequality can be rewritten as
\[ \Delta(G) + D(G) \leq n + 1 + \frac{\iota(G) - \Delta(G)}{n - 1}. \] (5.7)
If \( \Delta(G) \leq \iota(G) \), Inequality (5.7) is dominated by Inequality (5.3) and is thus valid. If \( \Delta(G) > \iota(G) \), then Lemma 5.4 gives \( \Delta(G) + D(G) \leq n \), which implies (5.7) because \( \Delta(G) \leq n - 1 \).

(ii) We now prove that, for \( n \geq 5 \) and \( n \) odd, Inequality (5.6) is facet defining. The following three graphs produce vectors which are linearly independent and satisfy Inequality (5.6) with equality: \( K_n, L_n \), and the graph on \( n \) nodes such that one of its nodes has degree \( n - 1 \) and the \( n - 1 \) other ones have degree \( n - 2 \). Notice that this last graph only exists for \( n \) odd.

On the contrary, as we will see at the end of this section, Inequality (5.6) is not facet defining when \( n \) is even. Before considering two more inequalities, we establish two lemmas.

**Lemma 5.6.** Let \( G \) be a connected graph with \( n \geq 4 \), \( D(G) \geq 3 \) and \( \Delta(G) + D(G) = n + 1 \). Then \( \iota(G) \geq 2\Delta(G) - 2 \).

Proof. We build upon the proof of Lemma 5.4. Let \( P = \{v_1, v_2, \ldots, v_{D(G)+1}\} \) be a diameter path containing some node \( v^* \) of degree \( \Delta(G) \). As in the proof of Lemma 5.4, we get \( v^* \in \{v_2, v_3, \ldots, v_{D(G)}\} \). Let \( V' \) be the set of exterior nodes. Note that an exterior node cannot be adjacent to both \( v_1 \) and \( v_{D(G)+1} \), because of our assumption \( D(G) \geq 3 \). Thus, \( V' \) is the disjoint union of the subset \( V_1 \) of exterior nodes adjacent to \( v_1 \), the subset \( V_2 \) of exterior nodes adjacent to \( v_{D(G)+1} \), and the subset \( V'' \) of all remaining exterior nodes. Consider three cases.

(a) Suppose \( V_1 \neq \emptyset \neq V_2 \). (This is possible only if \( D(G) = 3 \) or 4 because \( \Delta(G) + D(G) = n + 1 \) implies that all exterior nodes are adjacent to \( v^* \).) Consider the set \( P_1 \) of paths \( v_1, t, v^* \) with \( t \in V_1 \), and the set \( P_2 \) of paths \( v_{D(G)+1}, u, v^* \) with \( u \in V_2 \). The same argument as in the proof of Lemma 5.4 shows that the total irregularity computed along the paths from \( P_1 \), or from \( P_2 \), must be at least \( \Delta(G) - 1 \). Because \( V_1 \cap V_2 = \emptyset \), it is clear that any two paths in \( P_1 \cup P_2 \) have no common link. Thus
\[ \iota(G) \geq 2\Delta(G) - 2. \]

(b) Suppose \( V_1 \neq \emptyset \) and \( V_2 = \emptyset \) (the case where \( V_1 = \emptyset \) and \( V_2 \neq \emptyset \) can be treated along the same line). This implies \( d_{v_{D(G)+1}} = 1 \). Similarly to Case (a), the total irregularity along paths \( v_1, t, v^* \) with \( t \in V_1 \) is at least \( \Delta(G) - 1 \). Furthermore, the path \( Q = v_{D(G)+1}, v_{D(G)}^*, \ldots, v^* \) has no common link with those paths and it satisfies
\[ \iota(Q) \geq \Delta(G) - 1. \]
Hence
\[ \iota(G) \geq 2\Delta(G) - 2. \]

(c) Suppose \( V_1 = \emptyset = V_2 \). Then
\[ \iota(G) \geq \iota(\{v_1, v_2, \ldots, v^*\}) + \iota(\{v^*, \ldots, v_{D(G)}, v_{D(G)+1}\}) \geq 2\Delta(G) - 2. \]
Lemma 5.7. Let $G$ be a connected graph with $n$ even, $n \geq 4$, $D(G) = 2$, and $\Delta(G) = n - 1$. Then

$$\iota(G) \geq 2n - 4. \quad (5.8)$$

Proof. Let $k \geq 1$ be the number of nodes having degree $n - 1$. The links connecting the nodes of degree $n - 1$ to nodes of smaller degree lead to

$$\iota(G) \geq k(n - k). \quad (5.9)$$

If $2 \leq k \leq n - 2$, Inequality (5.8) follows from Inequality (5.9). Because the graph cannot be complete, the case $k = n - 1$ is impossible. It remains to consider the case $k = 1$.

Suppose $k = 1$, let $v$ be the unique node of degree $n - 1$ and let $\ell$ denote the number of nodes of degree $n - 2$. The contribution to $\iota(G)$ of the links connecting node $v$ to the $\ell$ nodes of degree $n - 2$ is $\ell$, and the contribution to $\iota(G)$ of the links connecting node $v$ to the $n - \ell - 1$ nodes of degree lower than $n - 2$ is at least $2(n - \ell - 1)$. Finally, the links connecting the $\ell$ nodes of degree $n - 2$ to the $n - \ell - 1$ nodes of degree lower than $n - 2$ contribute to $\iota(G)$ for at least $\ell(n - \ell - 2)$. Summing up, we obtain

$$\iota(G) \geq (\ell + 2)(n - \ell - 1).$$

If $0 \leq \ell \leq n - 3$, Inequality (5.8) follows from the above inequality. Notice that $\ell = n - 1$ is impossible because $n$ is even. Thus it remains to prove the result for $k = 1$ and $\ell = n - 2$.

Suppose $k = 1$ and $\ell = n - 2$. Then, there exists a unique node of degree $d < n - 2$ and

$$\iota(G) \geq (n - 2) + (n - 1 - d) + (d - 1)(n - 2 - d) \quad (5.10)$$

$$= n - 2 + d(n - 2 - d) + 1. \quad (5.11)$$

Because $d(n - 2 - d) \geq n - 3$ for $1 \leq d \leq n - 3$, the expression above leads to Inequality (5.8). \[\square\]

Proposition 5.8. The inequalities

$$2x_\Delta - x_\iota + 2xD \leq 2n \quad (5.12)$$

and

$$2(n - 1)x_\Delta - x_\iota + 2(n - 2)x_D \leq 2(n^2 - n - 1) \quad (5.13)$$

are facet defining for $P_{\Delta,\iota,D}^n$ when $n$ is even and $n \geq 4$.

Proof. (i) The validity of Inequality (5.12) can be easily proved: we show $2\Delta(G) - \iota + 2D \leq 2n$ for any connected graph $G$. If $G$ is regular, then (5.12) reduces to $\Delta(G) + D(G) \leq n$ which is always valid by Lemma 5.4. If $G$ is not regular, then $\iota(G) \geq 2$ and Inequality (5.12) is dominated by $2\Delta(G) + 2D(G) \leq 2n + 2$ which is true by Proposition 5.3.

The validity of Inequality (5.13) can be shown along the same line as in the proof of Proposition 5.3. Indeed, for a connected graph $G$, Inequality (5.13) is equivalent to

$$\Delta(G) + D(G) \leq n + 1 + \frac{2 + (\iota(G) - 2\Delta(G))}{2(n - 2)}. \quad (5.14)$$
Consider two cases.

(a) If $\Delta(G) + D(G) \leq n$, then (5.14) holds because $\Delta(G) \leq n - 1$ and $\epsilon \geq 0$ imply that the right hand side is bounded from below by $n$.

(b) Suppose $\Delta(G) + D(G) = n + 1$. Then the fact that the right hand side is bounded from below by $n + 1$ follows from Lemmas 5.6 and 5.7.

(ii) We now prove that the two inequalities in the statement are facet defining. For (5.13), three linearly independent vectors giving equality are provided by the graphs $K_n$, $L_n$ and the “boat” on $n$ nodes, i.e. the graph consisting of the path $L_{n-1}$ with an exterior node linked to its three consecutive middle nodes (see Figure 5.2). This last graph is well defined for $n \geq 4$ and $n$ even.

\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{boat.png}
\caption{The boat on 8 nodes.}
\end{figure}

For (5.12), replace the boat with the graph sketched in Figure 5.3.

\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{boat_mod.png}
\caption{A graph used in the proof of Proposition 5.8}
\end{figure}

This graph is defined for $n \geq 6$ and it has five nodes of degree 3, one node of degree 1, and all other nodes of degree 2. In case $n = 4$, use rather the complete graph minus one link. \[ \Box \]

Notice that the sum of Inequalities (5.12) and (5.13) is equal to twice (5.6). Consequently, the latter inequality does not define a facet for $n$ even.

In this section we have established some of the optimal inequalities among the diameter, the irregularity and the maximum degree of a connected graph. Even if we are not able this time to provide a complete description of the polytope of graph invariants, we have still shown that our method leads to nontrivial and interesting results. The problem of finding all optimal linear inequalities for the diameter, the irregularity and the maximum degree is left open.

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