Fibonacci Index and Stability Number of Graphs: a Polyhedral Study

Véronique Bruyère[*]   Hadrien Mélot[*,†]

November 10, 2008

Abstract. The Fibonacci index of a graph is the number of its stable sets. This parameter is widely studied and has applications in chemical graph theory. In this paper, we establish tight upper bounds for the Fibonacci index in terms of the stability number and the order of general graphs and connected graphs. Turán graphs frequently appear in extremal graph theory. We show that Turán graphs and a connected variant of them are also extremal for these particular problems. We also make a polyhedral study by establishing all the optimal linear inequalities for the stability number and the Fibonacci index, inside the classes of general and connected graphs of order n.

Keywords: Stable set; Fibonacci index; Merrifield-Simmons index; Turán graph; α-critical graph; GraPHedron.

---

1   Introduction

The Fibonacci index $F(G)$ of a graph G was introduced in 1982 by Prodinger and Tichy [21] as the number of stable sets in G. In 1989, Merrifield and Simmons [17] introduced independently this parameter in the chemistry literature[1]. They showed that there exist correlations between the boiling point and the Fibonacci index of a molecular graph. Since, the Fibonacci index has been widely studied, especially during the last few years. The majority of these recent results appeared in chemical graph theory [13, 14, 22, 24–26] and in extremal graph theory [10, 12, 18–20].

   In this literature, several results are bounds for $F(G)$ among graphs in particular classes. Lower and upper bounds inside the classes of general graphs, connected graphs, and trees are well known (see Section 2). Several authors give a characterization of trees with maximum Fibonacci index inside the class $\mathcal{T}(n, k)$ of trees with order n and a fixed parameter k. For example, Li et al. [14] determine such trees when k is the diameter; Heuberger and

---

[*]Department of Theoretical Computer Science, Université de Mons-Hainaut, Avenue du Champ de Mars 6, B-7000 Mons, Belgium.

[†]Chargé de Recherches F.R.S.-FNRS. Corresponding author. E-mail: `hadrien.melot@umh.ac.be`.

[1]The Fibonacci index is called the Fibonacci number by Prodinger and Tichy [21]. Merrifield and Simmons introduced it as the σ-index [17], also known as the Merrifield-Simmons index.

Wagner [10] when k is the maximum degree; and Wang et al. [26] when k is the number of pending vertices. Unicyclic graphs are also investigated in similar ways [18, 19, 25].

The Fibonacci index and the stability number of a graph are both related to stable sets. Hence, it is natural to use the stability number as a parameter to determine bounds for $F(G)$. Let $\mathcal{G}(n, \alpha)$ and $\mathcal{C}(n, \alpha)$ be the classes of – respectively general and connected – graphs with order n and stability number α. The lower bound for the Fibonacci index is known for graphs in these classes. Indeed, Pedersen and Vestergaard [19] give a simple proof to show that if $G \in \mathcal{G}(n, \alpha)$ or $G \in \mathcal{C}(n, \alpha)$, then $F(G) \geq 2^{\alpha} + n - \alpha$. Equality occurs if and only if G is a complete split graph (see Section 2). In this article, we determine upper bounds for $F(G)$ in the classes $\mathcal{G}(n, \alpha)$ and $\mathcal{C}(n, \alpha)$. In both cases, the bound is tight for every possible value of α and n and the extremal graphs are characterized.

A Turán graph is the union of disjoint balanced cliques. Turán graphs frequently appear in extremal graph theory. For example, the well-known Theorem of Turán [23] states that these graphs have minimum size inside $\mathcal{G}(n, \alpha)$. We show in Section 3 that Turán graphs have also maximum Fibonacci index inside $\mathcal{G}(n, \alpha)$. Observe that removing an edge in a graph strictly increases its Fibonacci index. Indeed, all existing stable sets remain and there is at least one more new stable set: the two vertices incident to the deleted edge. Therefore, we might have the intuition that the upper bound for $F(G)$ is a simple consequence of the Theorem of Turán. However, we show that it is not true (see Sections 2 and 6). The proof uses structural properties of α-critical graphs.

Graphs in $\mathcal{C}(n, \alpha)$ which maximize $F(G)$ are characterized in Section 4. We call them Turán-connected graphs since they are a connected variant of Turán graphs. It is interesting to note that these graphs again minimize the size inside $\mathcal{C}(n, \alpha)$. Hence, our results lead to questions about the relations between the Fibonacci index, the stability number, the size and the order of graphs. These questions are summarized in Section 6.

In Section 5, we further extend our results by a polyhedral study of the relations among the stability number and the Fibonacci index. Indeed, we state all the optimal linear inequalities for the stability number and the Fibonacci index, inside the classes of general and connected graphs of order n.

The major part of the results of this article has been published in Ref. [4].

2   Basic properties

In this section, we suppose that the reader is familiar with usual notions of graph theory (we refer to Berge [1] for more details). First, we fix our terminology and notation. We then recall the notion of α-critical graphs and give properties of such graphs, used in the next sections. We end with some basic properties of the Fibonacci index of a graph.

2.1 Notations

Let $G = (V, E)$ be a simple and undirected graph order $n(G) = |V|$ and size $m(G) = |E|$. For a vertex $v \in V(G)$, we denote by $N(v)$ the neighborhood of v; its closed neighborhood is defined as $\mathcal{N}(v) = N(v) \cup \{v\}$. The degree of a vertex v is denoted by $d(v)$ and the maximum degree of G by $\Delta(G)$. We use notation $G \simeq H$ when G and H are isomorphic graphs. The complement of G is denoted by $\overline{G}$.

The *stability number* $\alpha(G)$ of a graph G is the number of vertices of a maximum stable set of G. Clearly, $1 \leq \alpha(G) \leq n(G)$, and $1 \leq \alpha(G) \leq n(G) - 1$ when G is connected.

Definition 1. We denote by G^v the induced subgraph obtained by removing a vertex v from a graph G. Similarly, the graph $G^{N[v]}$ is the induced subgraph obtained by removing the closed neighborhood of v. Finally, the graph obtained by removing an edge e from G is denoted by G^e.

Classical graphs of order n are used in this article: the complete graph K_n, the path P_n, the cycle C_n, the star S_n (composed by one vertex adjacent to $n-1$ vertices of degree 1) and the complete split graph $\mathsf{CS}_{n,\alpha}$ (composed of a stable set of α vertices, a clique of $n - \alpha$ vertices and each vertex of the stable set is adjacent to each vertex of the clique). The complete split graph $\mathsf{CS}_{7,3}$ is depicted in Figure 1.

We also deeply study the two classes of Turán graphs and Turán-connected graphs. A *Turán graph* $\mathsf{T}_{n,\alpha}$ is a graph of order n and a stability number α such that $1 \leq \alpha \leq n$, that is defined as follows. It is the union of α disjoint balanced cliques (that is, such that their orders differ from at most one) [23]. These cliques have thus $\lceil \frac{n}{\alpha} \rceil$ or $\lfloor \frac{n}{\alpha} \rfloor$ vertices. We now define a *Turán-connected graph* $\mathsf{TC}_{n,\alpha}$ with n vertices and a stability number α where $1 \leq \alpha \leq n - 1$. It is constructed from the Turán graph $\mathsf{T}_{n,\alpha}$ with $\alpha - 1$ additional edges. Let v be a vertex of one clique of size $\lceil \frac{n}{\alpha} \rceil$, the additional edges link v and one vertex of each remaining cliques. Note that, for each of the two classes of graphs defined above, there is only one graph with given values of n and α, up to isomorphism.

Example 1. Figure 1 shows the Turán graph $\mathsf{T}_{7,3}$ and the Turán-connected graph $\mathsf{TC}_{7,3}$. When $\alpha = 1$, we observe that $\mathsf{T}_{n,1} \simeq \mathsf{TC}_{n,1} \simeq \mathsf{CS}_{n,1} \simeq \mathsf{K}_n$. When $\alpha = n$, we have $\mathsf{T}_{n,n} \simeq \mathsf{CS}_{n,n} \simeq \overline{\mathsf{K}_n}$, and when $\alpha = n - 1$, we have $\mathsf{TC}_{n,n-1} \simeq \mathsf{CS}_{n,n-1} \simeq \mathsf{S}_n$.
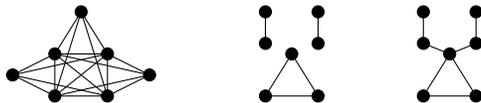
Figure 1: The graphs $\mathsf{CS}_{7,3}$, $\mathsf{T}_{7,3}$ and $\mathsf{TC}_{7,3}$

2.2 α-critical graphs

We recall the notion of α-critical graphs [7, 11, 15]. An edge e of a graph G is α-*critical* if $\alpha(G^e) > \alpha(G)$, otherwise it is called α-*safe*. A graph is said to be α-*critical* if all its edges are α-critical. By convention, a graph with no edge is also α-critical. These graphs play an important role in extremal graph theory [11], and also in our proofs.

Example 2. Simple examples of α-critical graphs are complete graphs and odd cycles. Turán graphs are also α-critical. On the contrary, Turán-connected graph are not α-critical, except when $\alpha = 1$.

We state some interesting properties of α-critical graphs.

Lemma 1. *Let G be an α-critical graph. If G is connected, then the graph G^v is connected for all vertices v of G.*

Proof. We use two known results on α-critical graphs (see, e.g., [15, Chapter 12]). If a vertex v of an α-critical graph has degree 1, then v and its neighbor w form a connected component of the graph. Every vertex of degree at least 2 in an α-critical graph is contained in a cycle.

Hence, by the first result, the minimum degree of G equals 2, except if $G \simeq \mathsf{K}_2$. Clearly G^v is connected by the second result or when $G \simeq \mathsf{K}_2$. $\qquad\square$

Lemma 2. *Let G be an α-critical graph. Let v be any vertex of G which is not isolated. Then,*

$$\alpha(G) = \alpha(G^v) = \alpha(G^{N[v]}) + 1.$$

Proof. Let $e = vw$ be an edge of G containing v. Then, there exist in G two maximum stable sets S and S', such that S contains v, but not w, and S' contains w, but not v (see, e.g., [15, Chapter 12]). Thus, $\alpha(G) = \alpha(G^v)$ due to the existence of S'. The set S avoids each vertex of $N(v)$. Hence, $S \setminus \{v\}$ is a stable set of the graph $G^{N[v]}$ of size $\alpha(G) - 1$. It is easy to check that this stable set is maximum. $\qquad\square$

2.3 Fibonacci index

Let us now recall the Fibonacci index of a graph [17, 21]. The *Fibonacci index $F(G)$* of a graph G is the number of all the stable sets in G, including the empty set. The following lemma about $F(G)$ is well-known (see [9, 14, 21]). It is used intensively through the article.

Lemma 3. *Let G be a graph.*

- *Let e be an edge of G, then $F(G) < F(G^e)$.*

- *Let v be a vertex of G, then $F(G) = F(G^v) + F(G^{N[v]})$.*

- *If G is the union of k disjoint graphs G_i, $1 \le i \le k$, then $F(G) = \prod_{i=1}^{k} F(G_i)$.*

4

Example 3. We have $F(\mathsf{K}_n) = n+1$, $F(\overline{\mathsf{K}_n}) = 2^n$, $F(\mathsf{S}_n) = 2^{n-1}+1$ and $F(\mathsf{P}_n) = f_{n+2}$ (recall that the sequence of Fibonacci numbers f_n is $f_0 = 0, f_1 = 1$ and $f_n = f_{n-1} + f_{n-2}$ for $n > 1$).

Prodinger and Tichy [21] give simple lower and upper bounds for the Fibonacci index. We recall these bounds in the next lemma.

Lemma 4. *Let G be a graph of order n.*

- *Then $n + 1 \leq F(G) \leq 2^n$ with equality if and only if $G \simeq \mathsf{K}_n$ (lower bound) and $G \simeq \overline{\mathsf{K}_n}$ (upper bound).*

- *If G is connected, then $n+1 \leq F(G) \leq 2^{n-1}+1$ with equality if and only if $G \simeq \mathsf{K}_n$ (lower bound) and $G \simeq \mathsf{S}_n$ (upper bound).*

- *If G is a tree, then $f_{n+2} \leq F(G) \leq 2^{n-1}+1$ with equality if and only if $G \simeq \mathsf{P}_n$ (lower bound) and $G \simeq \mathsf{S}_n$ (upper bound).*

We denote by $\mathcal{G}(n, \alpha)$ the class of general graphs with order n and stability number α; and by $\mathcal{C}(n, \alpha)$ the class of connected graphs with order n and stability number α. Pedersen and Vestergaard [19] characterize graphs with minimum Fibonacci index as indicated in the following theorem.

Theorem 5. *Let G be a graph inside $\mathcal{G}(n, \alpha)$ or $\mathcal{C}(n, \alpha)$, then*

$$F(G) \geq 2^\alpha + n - \alpha,$$

with equality if and only if $G \simeq \mathsf{CS}_{n,\alpha}$.

The aim of this article is the study of graphs with maximum Fibonacci index inside the two classes $\mathcal{G}(n, \alpha)$ and $\mathcal{C}(n, \alpha)$. The system GraPHedron [16] allows a formal framework to conjecture optimal relations among a set of graph invariants. Thanks to this system, graphs with maximum Fibonacci index inside each of the two previous classes have been computed for small values of n [8]. We observe that these graphs are isomorphic to Turán graphs for the class $\mathcal{G}(n, \alpha)$, and to Turán-connected graphs for the class $\mathcal{C}(n, \alpha)$. For the class $\mathcal{C}(n, \alpha)$, there is one exception when $n = 5$ and $\alpha = 2$: both the cycle C_5 and the graph $\mathsf{TC}_{5,2}$ have maximum Fibonacci index.

Recall that the classical Theorem of Turán [23] states that Turán graphs $\mathsf{T}_{n,\alpha}$ have minimum size inside $\mathcal{G}(n, \alpha)$. We might think that Turán graphs have maximum Fibonacci index inside $\mathcal{G}(n, \alpha)$ as a direct corollary of the Theorem of Turán and Lemma 3. This argument is not correct since removing an α-critical edge increases the stability number. Therefore, Lemma 3 only implies that graphs with maximum Fibonacci index inside $\mathcal{G}(n, \alpha)$ are α-critical graphs. In Section 6, we make further observations on the relations between the size and the Fibonacci index inside the classes $\mathcal{G}(n, \alpha)$ and $\mathcal{C}(n, \alpha)$.

There is another interesting property of Turán graphs related to stable sets. Byskov [5] establish that Turán graphs have maximum number of maximal stable sets inside $\mathcal{G}(n,\alpha)$. The Fibonacci index counts not only the maximal stable sets but all the stable sets. Hence, the fact that Turán graphs maximize $F(G)$ cannot be simply derived from the result of Byskov.

3 General graphs

In this section, we study graphs with maximum Fibonacci index inside the class $\mathcal{G}(n,\alpha)$. These graphs are said to be *extremal*. For fixed values of n and α, we show that there is one extremal graph up to isomorphism, the Turán graph $\mathsf{T}_{n,\alpha}$ (see Theorem 8).

Before establishing this result, we need some auxiliary results. We denote by $f_{\mathsf{T}}(n,\alpha)$ the Fibonacci index of the Turán graph $\mathsf{T}_{n,\alpha}$. By Lemma 3, its value is equal to

$$f_{\mathsf{T}}(n,\alpha) = \left(\left\lceil \frac{n}{\alpha} \right\rceil + 1\right)^p \left(\left\lfloor \frac{n}{\alpha} \right\rfloor + 1\right)^{\alpha-p},$$

where $p = (n \mod \alpha)$. We have also the following inductive formula.

Lemma 6. *Let n and α be integers such that $1 \leq \alpha \leq n$. Then*

$$f_{\mathsf{T}}(n,\alpha) = \begin{cases} n+1 & if \quad \alpha = 1, \\ 2^n & if \quad \alpha = n, \\ f_{\mathsf{T}}(n-1,\alpha) + f_{\mathsf{T}}(n - \left\lceil \frac{n}{\alpha} \right\rceil, \alpha - 1) & if \quad 2 \leq \alpha \leq n-1. \end{cases}$$

Proof. The cases $\alpha = 1$ and $\alpha = n$ are trivial (see Example 3). Suppose $2 \leq \alpha \leq n-1$. Let v be a vertex of $\mathsf{T}_{n,\alpha}$ with maximum degree. Thus v is in a $\left\lceil \frac{n}{\alpha} \right\rceil$-clique. As $\alpha < n$, the vertex v is not isolated. Therefore $\mathsf{T}_{n,\alpha}^v \simeq \mathsf{T}_{n-1,\alpha}$. As $\alpha \geq 2$, the graph $\mathsf{T}_{n,\alpha}^{N[v]}$ has at least one vertex, and $\mathsf{T}_{n,\alpha}^{N[v]} \simeq \mathsf{T}_{n-\left\lceil \frac{n}{\alpha} \right\rceil, \alpha-1}$. By Lemma 3, we obtain

$$f_{\mathsf{T}}(n,\alpha) = f_{\mathsf{T}}(n-1,\alpha) + f_{\mathsf{T}}(n - \left\lceil \frac{n}{\alpha} \right\rceil, \alpha - 1). \qquad \square$$

A consequence of Lemma 6 is that $f_{\mathsf{T}}(n-1,\alpha) < f_{\mathsf{T}}(n,\alpha)$. Indeed, the cases $\alpha = 1$ and $\alpha = n$ are trivial, and the term $f_{\mathsf{T}}(n - \left\lceil \frac{n}{\alpha} \right\rceil, \alpha - 1)$ is always strictly positive when $2 \leq \alpha \leq n-1$.

Corollary 7. *The function $f_{\mathsf{T}}(n,\alpha)$ is strictly increasing in n when α is fixed.*

We now state the upper bound on the Fibonacci index of graphs in the class $\mathcal{G}(n,\alpha)$.

Theorem 8. *Let G be a graph of order n with a stability number α, then*

$$F(G) \leq f_{\mathsf{T}}(n,\alpha),$$

with equality if and only if $G \simeq \mathsf{T}_{n,\alpha}$.

6

Proof. The cases $\alpha = 1$ and $\alpha = n$ are straightforward. Indeed $G \simeq \mathsf{T}_{n,1}$ when $\alpha = 1$, and $G \simeq \mathsf{T}_{n,n}$ when $\alpha = n$. We can assume that $2 \leq \alpha \leq n-1$, and thus $n \geq 3$. We now prove by induction on n that if G is extremal, then it is isomorphic to $\mathsf{T}_{n,\alpha}$.

The graph G is α-critical. Otherwise, there exists an edge $e \in E(G)$ such that $\alpha(G) = \alpha(G^e)$, and by Lemma 3, $F(G) < F(G^e)$. This is a contradiction with G being extremal.

Let us compute $F(G)$ thanks to Lemma 3. Let $v \in V(G)$ of maximum degree Δ. The vertex v is not isolated since $\alpha < n$. Thus by Lemma 2, $\alpha(G^v) = \alpha$ and $\alpha(G^{N[v]}) = \alpha - 1$. On the other hand, If χ is the chromatic number of G, it is well-known that $n \leq \chi \cdot \alpha$ (see, e.g., Berge [1]), and that $\chi \leq \Delta + 1$ (see Brooks [3]). It follows that

$$n(G^{N[v]}) = n - \Delta - 1 \leq n - \left\lceil \frac{n}{\alpha} \right\rceil. \tag{1}$$

Note that $n(G^{N[v]}) \geq 1$ since $\alpha \geq 2$.

We can apply the induction hypothesis on the graphs G^v and $G^{N[v]}$. We obtain

$$
\begin{array}{rcll}
f_{\mathsf{T}}(n,\alpha) & \leq & F(G) & \text{as } G \text{ is extremal,} \\
& = & F(G^v) + F(G^{N[v]}) & \text{by Lemma 3,} \\
& \leq & f_{\mathsf{T}}(n(G^v), \alpha(G^v)) + f_{\mathsf{T}}(n(G^{N[v]}), \alpha(G^{N[v]})) & \text{by induction,} \\
& = & f_{\mathsf{T}}(n-1, \alpha) + f_{\mathsf{T}}(n - \Delta - 1, \alpha - 1) & \\
& \leq & f_{\mathsf{T}}(n-1, \alpha) + f_{\mathsf{T}}(n - \left\lceil \frac{n}{\alpha} \right\rceil, \alpha - 1) & \text{by Eq. (1) and Corollary 7,} \\
& = & f_{\mathsf{T}}(n, \alpha) & \text{by Lemma 6.}
\end{array}
$$

Hence equality holds everywhere. In particular, by induction, the graphs G^v, $G^{N[v]}$ are extremal, and $G^v \simeq \mathsf{T}_{n-1,\alpha}$, $G^{N[v]} \simeq \mathsf{T}_{n-\lceil \frac{n}{\alpha} \rceil, \alpha-1}$. Coming back to G from G^v and $G^{N[v]}$ and recalling that v has maximum degree, it follows that $G \simeq \mathsf{T}_{n,\alpha}$. $\qquad \square$

Corollary 7 states that $f_{\mathsf{T}}(n, \alpha)$ is increasing in n. It was an easy consequence of Lemma 6. The function $f_{\mathsf{T}}(n, \alpha)$ is also increasing in α. Theorem 8 can be used to prove this fact easily as shown now.

Corollary 9. *The function $f_{\mathsf{T}}(n, \alpha)$ is strictly increasing in α when n is fixed.*

Proof. Suppose $2 \leq \alpha \leq n-1$. By Lemma 4 it is clear that $f_{\mathsf{T}}(n, 1) < f_{\mathsf{T}}(n, \alpha) < f_{\mathsf{T}}(n, n)$. Now, let e be an edge of $\mathsf{T}_{n,\alpha}$. Clearly $\alpha(\mathsf{T}_{n,\alpha}^e) = \alpha + 1$. Moreover, by Lemma 3 and Theorem 8,

$$F(\mathsf{T}_{n,\alpha}) < F(\mathsf{T}_{n,\alpha}^e) < F(\mathsf{T}_{n,\alpha+1}).$$

Therefore, $f_{\mathsf{T}}(n, \alpha) < f_{\mathsf{T}}(n, \alpha + 1)$. $\qquad \square$

4 Connected graphs

We now consider graphs with maximum Fibonacci index inside the class $\mathcal{C}(n,\alpha)$. Such graphs are called *extremal*. If G is connected, the bound of Theorem 8 is clearly not tight, except when $\alpha = 1$, that is, when G is a complete graph. We are going to prove that there is one extremal graph up to isomorphism, the Turán-connected graph $\mathsf{TC}_{n,\alpha}$, with the exception of the cycle C_5 (see Theorem 12). First, we need preliminary results and definitions to prove this theorem.

We denote by $f_{\mathsf{TC}}(n,\alpha)$ the Fibonacci index of the Turán-connected graph $\mathsf{TC}_{n,\alpha}$. An inductive formula for its value is given in the next lemma.

Lemma 10. *Let n and α be integers such that $1 \le \alpha \le n - 1$. Then*

$$f_{\mathsf{TC}}(n,\alpha) = \begin{cases} n+1 & if \quad \alpha = 1, \\ 2^{n-1} + 1 & if \quad \alpha = n-1, \\ f_{\mathsf{T}}(n-1,\alpha) + f_{\mathsf{T}}(n',\alpha') & if \quad 2 \le \alpha \le n-2, \end{cases}$$

where $n' = n - \left\lceil \frac{n}{\alpha} \right\rceil - \alpha + 1$ and $\alpha' = \min(n', \alpha - 1)$.

Proof. The cases $\alpha = 1$ and $\alpha = n - 1$ are trivial by Lemma 4. Suppose now that $2 \le \alpha \le n - 2$. Let v be a vertex of maximum degree in $\mathsf{TC}_{n,\alpha}$. We apply Lemma 3 to compute $F(\mathsf{TC}_{n,\alpha})$. Observe that the graphs $\mathsf{TC}_{n,\alpha}^v$ and $\mathsf{TC}_{n,\alpha}^{N[v]}$ are both Turán graphs when $2 \le \alpha \le n - 2$.

The graph $\mathsf{TC}_{n,\alpha}^v$ is isomorphic to $\mathsf{T}_{n-1,\alpha}$. Let us show that $\mathsf{TC}_{n,\alpha}^{N[v]}$ is isomorphic to $\mathsf{T}_{n',\alpha'}$. By definition of a Turán-connected graph, $d(v)$ is equal to $\left\lceil \frac{n}{\alpha} \right\rceil + \alpha - 2$. Thus

$$n(\mathsf{TC}_{n,\alpha}^{N[v]}) = n - d(v) - 1 = n'.$$

If $\alpha < \frac{n}{2}$, then $\mathsf{TC}_{n,\alpha}$ has a clique of order at least 3 and $\alpha(\mathsf{TC}_{n,\alpha}^{N[v]}) = \alpha - 1 \le n'$. Otherwise, $\mathsf{TC}_{n,\alpha}^{N[v]} \simeq \overline{\mathsf{K}_{n'}}$ and $\alpha(\mathsf{TC}_{n,\alpha}^{N[v]}) = n' \le \alpha - 1$. Therefore $\alpha(\mathsf{TC}_{n,\alpha}^{N[v]}) = \min(n', \alpha - 1)$ in both cases.

By Lemma 3, these observations leads to

$$f_{\mathsf{TC}}(n,\alpha) = f_{\mathsf{T}}(n-1,\alpha) + f_{\mathsf{T}}(n',\alpha'). \qquad \square$$

Definition 2. A *bridge* in a connected graph G is an edge $e \in E(G)$ such that the graph G^e is no more connected. To a bridge $e = v_1 v_2$ of G which is α-safe, we associate a *decomposition* $\mathcal{D}(G_1, v_1, G_2, v_2)$ such that $v_1 \in V(G_1)$, $v_2 \in V(G_2)$, and G_1, G_2 are the two connected components of G^e. A decomposition is said to be *α-critical* if G_1 is α-critical.

Lemma 11. *Let G be a connected graph. If G is extremal, then either G is α-critical or G has an α-critical decomposition.*

8

Proof. We suppose that G is not α-critical and we show that it must contain an α-critical decomposition.

Let e be an α-safe edge of G. Then e must be a bridge. Otherwise, the graph G^e is connected, has the same order and stability number as G and satisfies $F(G^e) > F(G)$ by Lemma 3. This is a contradiction with G being extremal. Therefore G contains at least one α-safe bridge defining a decomposition of G.

Let us choose a decomposition $\mathcal{D}(G_1, v_1, G_2, v_2)$ such that G_1 is of minimum order. Then, G_1 is α-critical. Otherwise, G_1 contains an α-safe bridge $e' = w_1 w_2$, since the edges of G are α-critical or α-safe bridges by the first part of the proof. Let $\mathcal{D}(H_1, w_1, H_2, w_2)$ be the decomposition of G defined by e', such that $v_1 \in V(H_2)$. Then $n(H_1) < n(G_1)$, which is a contradiction. Hence the decomposition $\mathcal{D}(G_1, v_1, G_2, v_2)$ is α-critical. $\square$

Theorem 12. *Let G be a connected graph of order n with a stability number α, then*

$$F(G) \leq f_{\mathsf{TC}}(n, \alpha),$$

with equality if and only if $G \simeq \mathsf{TC}_{n,\alpha}$ when $(n, \alpha) \neq (5, 2)$, and $G \simeq \mathsf{TC}_{5,2}$ or $G \simeq \mathsf{C}_5$ when $(n, \alpha) = (5, 2)$.

Proof. We prove by induction on n that if G is extremal, then it is isomorphic to $\mathsf{TC}_{n,\alpha}$ or C_5. To handle more easily the general case of the induction (in a way to avoid the extremal graph C_5), we consider all connected graphs with up to 6 vertices as the basis of the induction. For these basic cases, we refer to the report of an exhaustive automated verification [8]. We thus suppose that $n \geq 7$.

We know by Lemma 11 that either G has an α-critical decomposition or G is α-critical. We consider now these two situations.

1) G has an α-critical decomposition. We prove in three steps that $G \simeq \mathsf{TC}_{n,\alpha}$: ($i$) We establish that for every decomposition $\mathcal{D}(G_1, v_1, G_2, v_2)$, the graph G_i is extremal and is isomorphic to a Turán-connected graph such that $d(v_i) = \Delta(G_i)$, for $i = 1, 2$. (ii) We show that if such a decomposition is α-critical, then G_1 is a clique. (iii) We prove that G is itself isomorphic to a Turán-connected graph.

(i) For the first step, let $\mathcal{D}(G_1, v_1, G_2, v_2)$ be a decomposition of G, n_1 be the order of G_1, and α_1 its stability number. We prove that $G_1 \simeq \mathsf{TC}_{n_1, \alpha_1}$ such that $d(v_1) = \Delta(G_1)$. The argument is identical for G_2. By Lemma 3, we have

$$F(G) = F(G_1)F(G_2^{v_2}) + F(G_1^{v_1})F(G_2^{N[v_2]}).$$

By the induction hypothesis, $F(G_1) \leq f_{\mathsf{TC}}(n_1, \alpha_1)$. The graph $G_1^{v_1}$ has an order $n_1 - 1$ and a stability number $\leq \alpha_1$. Hence by Theorem 8 and Corollary 9, $F(G_1^{v_1}) \leq f_{\mathsf{T}}(n_1 - 1, \alpha_1)$. It follows that

$$F(G) \leq f_{\mathsf{TC}}(n_1, \alpha_1)F(G_2^{v_2}) + f_{\mathsf{T}}(n_1 - 1, \alpha_1)F(G_2^{N[v_2]}). \tag{2}$$

As G is supposed to be extremal, equality occurs. It means that $G_1^{v_1} \simeq \mathsf{T}_{n_1-1,\alpha_1}$ and G_1 is extremal. If G_1 is isomorphic to C_5, then $n_1 = 5$, $\alpha_1 = 2$ and $F(G_1) = f_{\mathsf{TC}}(5,2)$. However, $F(G_1^{v_1}) = F(\mathsf{P}_4) < f_{\mathsf{T}}(4,2)$. By (2), this leads to a contradiction with G being extremal. Thus, G_1 must be isomorphic to $\mathsf{TC}_{n_1,\alpha_1}$. Moreover, v_1 is a vertex of maximum degree of G_1. Otherwise, $G_1^{v_1}$ cannot be isomorphic to the graph $\mathsf{T}_{n_1-1,\alpha_1}$.

(ii) The second step is easy. Let $\mathcal{D}(G_1,v_1,G_2,v_2)$ be an α-critical decomposition of G, that is, G_1 is α-critical. By (i), G_1 is isomorphic to a Turán-connected graph. The complete graph is the only Turán-connected graph which is α-critical. Therefore, G_1 is a clique.

(iii) We now suppose that G has an α-critical decomposition $\mathcal{D}(G_1,v_1,G_2,v_2)$ and we show that $G \simeq \mathsf{TC}_{n,\alpha}$. Let n_1 be the order of G_1 and α_1 its stability number. As v_1v_2 is an α-safe bridge, it is clear that $n(G_2) = n - n_1$ and $\alpha(G_2) = \alpha - \alpha_1$. By ($i$) and ($ii$), G_1 is a clique (and thus $\alpha_1 = 1$), $G_2 \simeq \mathsf{TC}_{n-n_1,\alpha-1}$, and v_2 is a vertex of maximum degree in G_2.

If $\alpha = 2$, then G_2 is also a clique in G. By Lemma 3 and the fact that $F(\mathsf{K}_n) = n+1$ we have,
$$\begin{aligned} F(G) &= F(G^{v_1}) + F(G^{N[v_1]}) \\ &= n_1(n - n_1 + 1) + (n - n_1) = n + n\,n_1 - n_1^2. \end{aligned}$$

When n is fixed, this function is maximized when $n_1 = \frac{n}{2}$. That is, when G_1 and G_2 are balanced cliques. This appears if and only if $G \simeq \mathsf{TC}_{n,2}$.

Thus we suppose that $\alpha \geq 3$. In other words, G contains at least three cliques: the clique G_1 of order n_1; the clique H containing v_2 and a clique H' in G_2 linked to H by an α-safe bridge v_2v_3. Let $k = \frac{n-n_1}{\alpha-1}$, then the order of H is $\lceil k \rceil$ and the order of H' is $\lceil k \rceil$ or $\lfloor k \rfloor$ (recall that $G_2 \simeq \mathsf{TC}_{n-n_1,\alpha-1}$). These cliques are represented in Figure 2.
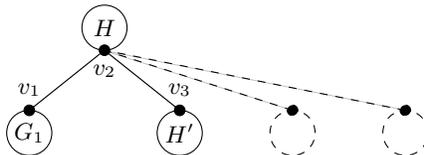

Figure 2: Cliques in the graph G

To prove that G is isomorphic to a Turán-connected graph, it remains to show that the clique G_1 is balanced with the cliques H and H'. We consider the decomposition defined by the α-safe bridge v_2v_3. By (i), G_1 and H are cliques of a Turán-connected graph, and H is a clique with maximum order in this graph (recall that v_2 is a vertex of maximum degree in G_2). Therefore $\lceil k \rceil - 1 \leq n_1 \leq \lceil k \rceil$, showing that G_1 is balanced with H and H'.

2) G is α-critical. Under this hypothesis, we prove that G is a complete graph, and thus is isomorphic to a Turán-connected graph.

10

Suppose that G is not complete. Let v be a vertex of G with a maximum degree $d(v) = \Delta$. As G is connected and α-critical, the graph G^v is connected by Lemma 1. By Lemma 2, $\alpha(G^v) = \alpha$ and $\alpha(G^{N[v]}) = \alpha - 1$. Moreover, $n(G^v) = n - 1$ and $n(G^{N[v]}) = n - \Delta - 1$. By the induction hypothesis and Theorem 8, we get

$$F(G) = F(G^v) + F(G^{N[v]}) \leq f_{\mathsf{TC}}(n - 1, \alpha) + f_{\mathsf{T}}(n - \Delta - 1, \alpha - 1).$$

Therefore, G is extremal if and only if $G^{N[v]} \simeq \mathsf{T}_{n-\Delta-1,\alpha-1}$ and G^v is extremal. However, G^v is not isomorphic to C_5 as $n \geq 7$. Thus $G^v \simeq \mathsf{TC}_{n-1,\alpha}$.

So, the graph G is composed by the graph $G^v \simeq \mathsf{TC}_{n-1,\alpha}$ and an additional vertex v connected to $\mathsf{TC}_{n-1,\alpha}$ by Δ edges.

There must be an edge between v and a vertex v' of maximum degree in G^v, otherwise $G^{N[v]}$ is not isomorphic to a Turán graph. The vertex v' is adjacent to $\left\lceil \frac{n-1}{\alpha} \right\rceil + \alpha - 2$ vertices in G^v and it is adjacent to v, that is,

$$d(v') = \left\lceil \frac{n-1}{\alpha} \right\rceil + \alpha - 1.$$

It follows that

$$\Delta \geq d(v') > \left\lceil \frac{n-1}{\alpha} \right\rceil \tag{3}$$

as G is not a complete graph.

On the other hand, v is adjacent to each vertex of some clique H of G^v since $G^{N[v]}$ has a stability number $\alpha - 1$. As this clique has order at most $\left\lceil \frac{n-1}{\alpha} \right\rceil$, v must be adjacent to a vertex $w \notin H$ by (3).

We observe that the edge vw is α-safe. This is impossible as G is α-critical. It follows that G is a complete graph and the proof is completed. $\qquad\square$

The study of the maximum Fibonacci index inside the class $\mathcal{T}(n, \alpha)$ of trees with order n and stability number α is strongly related to the study done in this section for the class $\mathcal{C}(n, \alpha)$. Indeed, due to the fact that trees are bipartite, a tree in $\mathcal{T}(n, \alpha)$ has always a stability number $\alpha \geq \frac{n}{2}$. Moreover, the Turán-connected graph $\mathsf{TC}_{n,\alpha}$ is a tree when $\alpha \geq \frac{n}{2}$. Therefore, the upper bound on the Fibonacci index for connected graphs is also valid for trees. We thus get the next corollary with in addition the exact value of $f_{\mathsf{TC}}(n, \alpha)$.

Corollary 13. *Let G be a tree of order n with a stability number α, then*

$$F(G) \leq 3^{n-\alpha-1} 2^{2\alpha-n+1} + 2^{n-\alpha-1},$$

with equality if and only if $G \simeq \mathsf{TC}_{n,\alpha}$.

Proof. It remains to compute the exact value of $f_{\mathsf{TC}}(n, \alpha)$. When $\alpha \geq \frac{n}{2}$, the graph $\mathsf{TC}_{n,\alpha}$ is composed by one central vertex v of degree α and α pending paths of length 1 or 2 attached

to v. An extremity of a pending path of length 2 is a vertex w such that $w \notin \mathcal{N}(v)$. Thus there are $x = n - \alpha - 1$ pending paths of length 2 since $\mathcal{N}(v)$ has size $\alpha + 1$, and there are $y = \alpha - x = 2\alpha - n + 1$ pending paths of length 1. We apply Lemma 3 on v to get

$$f_{\mathsf{TC}}(n, \alpha) = F(\mathsf{K}_2)^x F(\mathsf{K}_1)^y + F(\mathsf{K}_1)^x = 3^x 2^y + 2^x. \qquad \square$$

We conclude this section by showing that the function $f_{\mathsf{TC}}(n, \alpha)$ is strictly increasing in n and α, as already stated for the function $f_{\mathsf{T}}(n, \alpha)$ (see Corollaries 7 and 9).

Proposition 14. *The function $f_{\mathsf{TC}}(n, \alpha)$ is strictly increasing in n and α.*

Proof. We first prove that $f_{\mathsf{TC}}(n, \alpha)$ is strictly increasing in n when α is fixed. The cases $\alpha = 1$ and $\alpha = n - 1$ are obvious by Lemma 10 and we suppose that $2 \leq \alpha \leq n - 2$. Let $n' = n - \lceil \frac{n}{\alpha} \rceil - \alpha + 1$ and $\alpha' = \min(n', \alpha - 1)$. Also, we note $n'' = n + 1 - \lceil \frac{n+1}{\alpha} \rceil - \alpha + 1$ and $\alpha'' = \min(n'', \alpha - 1)$. Observe that $n' \leq n''$ and $\alpha' \leq \alpha''$. We have

$$
\begin{aligned}
f_{\mathsf{TC}}(n, \alpha) &= f_{\mathsf{T}}(n - 1, \alpha) + f_{\mathsf{T}}(n', \alpha') &\text{by Lemma 10,} \\
&< f_{\mathsf{T}}(n, \alpha) + f_{\mathsf{T}}(n'', \alpha'') &\text{by Corollaries 7 and 9,} \\
&= f_{\mathsf{TC}}(n + 1, \alpha) &\text{by Lemma 10.}
\end{aligned}
$$

Therefore, $f_{\mathsf{TC}}(n, \alpha) < f_{\mathsf{TC}}(n + 1, \alpha)$.

We now prove that $f_{\mathsf{TC}}(n, \alpha)$ is strictly increasing in α when n is fixed. Let $2 \leq \alpha \leq n - 2$. Obviously, $f_{\mathsf{TC}}(n, 1) < f_{\mathsf{TC}}(n, \alpha) < f_{\mathsf{TC}}(n, n - 1)$ by Lemma 4. We consider two cases.

a) If $\alpha < \frac{n}{2}$, then $\mathsf{TC}_{n,\alpha}$ contains at least one clique H of size at least 3 and the remaining cliques are of size at least 2. Suppose that G is the graph obtained from $\mathsf{TC}_{n,\alpha}$ by removing an edge inside H. Then, G is connected and $\alpha(G) = \alpha + 1$. Moreover, Lemma 3 and Theorem 12 ensure that $f_{\mathsf{TC}}(n, \alpha) < F(G) < f_{\mathsf{TC}}(n, \alpha + 1)$ and the result follows.

b) Suppose now that $\alpha \geq \frac{n}{2}$. In this case, $\mathsf{TC}_{n,\alpha}$ and $\mathsf{TC}_{n,\alpha+1}$ are trees. Let $x = n - \alpha - 1$, $x' = n - \alpha - 2$, $y = 2\alpha - n + 1$, and $y' = 2\alpha - n + 3$. Then,

$$
\begin{aligned}
f_{\mathsf{TC}}(n, \alpha + 1) - f_{\mathsf{TC}}(n, \alpha) &= 3^{x'} 2^{y'} + 2^{x'} - 3^x 2^y - 2^x &\text{by Corollary 13,} \\
&= 3^{x-1} 2^y - 2^{x-1}.
\end{aligned}
$$

As $\alpha \leq n - 2$, we have that $x - 1 \geq 0$. Thus, $2^{x-1} \leq 3^{x-1}$. Moreover, as $\alpha \geq \frac{n}{2}$, we have that $y \geq 0$ and thus $2^y \geq 1$. It follows that $3^{x-1} 2^y - 2^{x-1} \geq 0$. The case of equality with 0 happens when both $x - 1 = 0$ and $y = 0$, that is, when $\alpha = 1$. This never holds since $\alpha \geq 2$. Therefore $f_{\mathsf{TC}}(n, \alpha)$ is strictly increasing in α. $\qquad \square$

5 Polyhedral study

In the previous sections, we have stated that the graphs with maximum Fibonacci index inside the classes $\mathcal{G}(n, \alpha)$ and $\mathcal{C}(n, \alpha)$ are isomorphic to Turán graphs and Turán-connected graphs respectively (see Theorems 8 and 12). These results have been suggested thanks to the system GraPHedron [8].

In this section, we further push the use of the system GraPHedron as outlined in [16]. Indeed, this framework allows to suggest the set of all optimal linear inequalities among the stability number and the Fibonacci index for graphs inside the class $\mathcal{G}(n)$ of general graphs of order n and the class $\mathcal{C}(n)$ of connected graphs of order n. That is, it allows to determine for small values of n the complete description of the polytopes

$$\mathcal{P}_{\mathcal{G}(n)} = \operatorname{conv} \left\{ (x, y) \mid \exists G \in \mathcal{G}(n), \alpha(G) = x, F(G) = y \right\}, \tag{4}$$

$$\mathcal{P}_{\mathcal{C}(n)} = \operatorname{conv} \left\{ (x, y) \mid \exists G \in \mathcal{C}(n), \alpha(G) = x, F(G) = y \right\}, \tag{5}$$
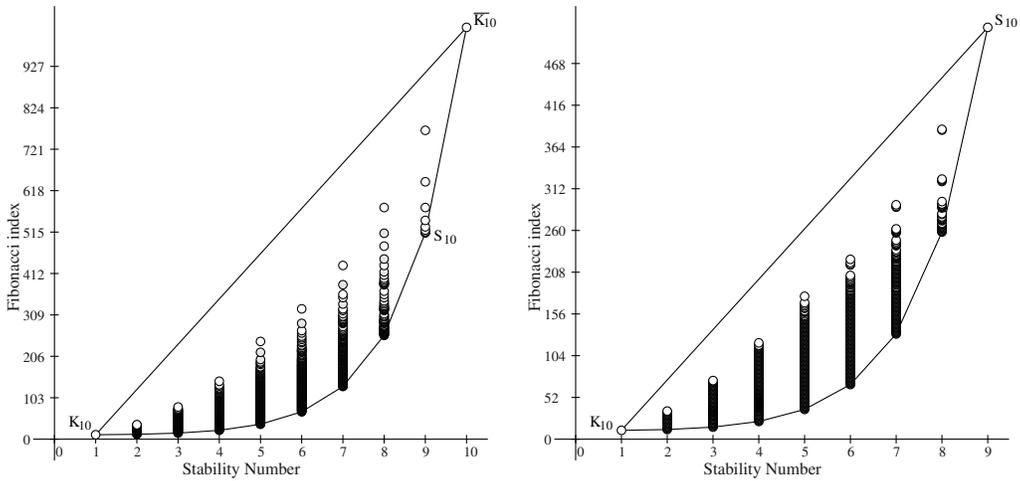
where *conv* denotes the convex hull.

Figure 3: The polytopes $\mathcal{P}_{\mathcal{G}(10)}$ (left) and $\mathcal{P}_{\mathcal{C}(10)}$ (right)

For example, Figure 3 shows the polytopes $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$ when $n = 10$, as given in the reports created by GraPHedron [8]. In these representations, we associate to a point (x, y) the set of all graphs with a stability number x and a Fibonacci index y, and we say that the point (x, y) *corresponds* to these graphs. For instance, in Figure 3, the point $(1, 11)$ corresponds to the graph K_{10}, whereas the point $(9, 2^9 + 1)$ corresponds to the graph S_{10}.

13

In this section, we make a polyhedral study in a way to give a complete description of the polytopes $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$ for all (sufficiently large) values of n. More precisely, we are going to describe the *facet defining inequalities* of both polytopes $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$, that is, their minimal system of linear inequalities. Let us fix some notation:

$$\mathsf{L}_n(x) = \frac{2^n - n - 1}{n - 1}(x - 1) + n + 1,$$

$$\mathsf{L}'_n(x) = \frac{2^{n-1} - n}{n - 2}(x - 1) + n + 1.$$

The following Theorems 15 and 16 give the complete description of $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$. These theorems will be proved at the end of this section, after some preliminary results.

Theorem 15. *Let $n \geq 5$. Then the polytope $\mathcal{P}_{\mathcal{G}(n)}$ has n facets defined by the inequalities*

$$y \;\geq\; \left(2^k - 1\right)x + 2^k(1 - k) + n, \quad for\ k = 1, 2, \ldots, n - 1, \tag{6}$$

$$y \;\leq\; \mathsf{L}_n(x). \tag{7}$$

Theorem 16. *Let $n \geq 8$. Then the polytope $\mathcal{P}_{\mathcal{C}(n)}$ has $n-1$ facets defined by the inequalities*

$$y \;\geq\; \left(2^k - 1\right)x + 2^k(1 - k) + n, \quad for\ k = 1, 2, \ldots, n - 2, \tag{8}$$

$$y \;\leq\; \mathsf{L}'_n(x). \tag{9}$$

We first make some comments. In Figure 4, the two polytopes $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$ are drawn together. This gives a graphical summary of the main results stated in Theorems 5, 8, 12, 15 and 16:

- black points correspond to Turán graphs and have maximum y-value among general graphs by Theorem 8;

- grey points correspond to Turán-connected graphs and have maximum y-value among connected graphs by Theorem 12;

- white points correspond to complete split graphs and have minimum y-value among general and connected graphs by Theorem 5;

- the n facets of $\mathcal{P}_{\mathcal{G}(n)}$ are the $n - 1$ lines joining two consecutive points corresponding to complete split graphs, and the line $y = \mathsf{L}_n(x)$ joining the two points corresponding to K_n and $\overline{\mathsf{K}_n}$ (see Theorem 15);

- the $n-1$ facets of $\mathcal{P}_{\mathcal{C}(n)}$ are the $n-2$ lines joining two consecutive points corresponding to (connected) complete split graphs, and the line $y = \mathsf{L}'_n(x)$ joining the two points corresponding to K_n and S_n (see Theorem 16).
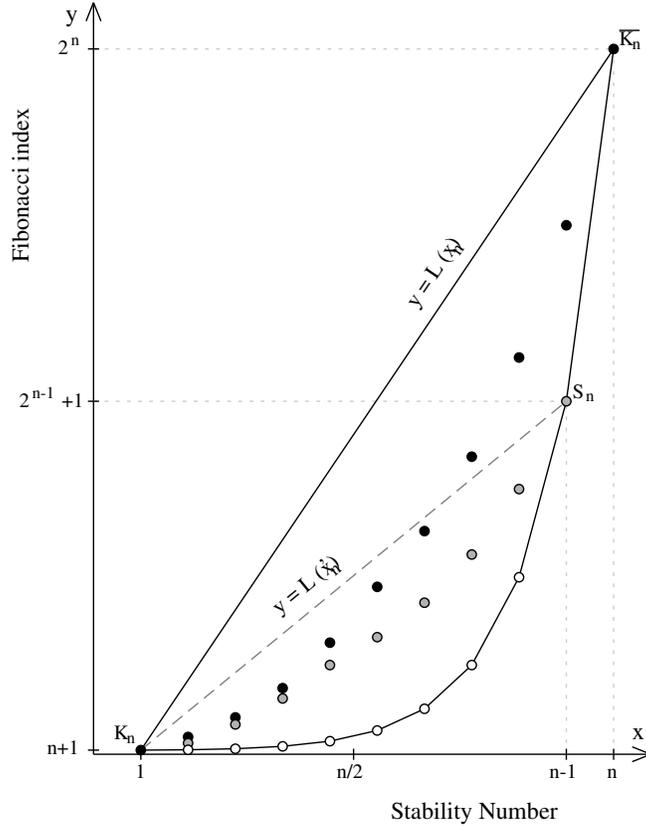
14

Figure 4: Representation of $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$ together

In the next lemma, we establish the inequalities (7) and (9).

Lemma 17. *The inequality*

$$y \geq \left(2^k - 1\right) x + 2^k(1 - k) + n, \tag{10}$$

defines a facet of $\mathcal{P}_{\mathcal{G}(n)}$ for $k = 1, 2, \ldots, n - 1$, and a facet of $\mathcal{P}_{\mathcal{C}(n)}$ for $k = 1, 2, \ldots, n - 2$.

Proof. We know by Theorem 5 that the points which have minimum y-values are those corresponding to complete split graphs. These points are

$$(x, \; 2^x + n - x),$$

which are convexly independent as the function $2^x + n - x$ is strictly convex in x. Therefore these points are vertices of $\mathcal{P}_{\mathcal{G}(n)}$ and $\mathcal{P}_{\mathcal{C}(n)}$, for $x = 1, 2, \ldots, n - 1$, and $x = 1, 2, \ldots, n - 2$,

15

respectively. Moreover, there can be no other polytope vertices between two consecutive points because x is increasing by step of 1, and there exists a complete split graph for each possible value of x.

Ineq. (10) can then be derived by computing the equation of the line passing by two consecutive points $\left(k,\ 2^k + n - k\right)$ and $\left(k+1,\ 2^{k+1} + n - k - 1\right)$. It is obvious that Ineq. (10) is facet defining since these points are two independent polytope vertices. □

We now consider the class $\mathcal{G}(n)$ and study in more details how points (x, y) corresponding to graphs G with $\alpha(G) = x$ and $F(G) = y$ are situated with respect to the line $y = \mathsf{L}_n(x)$.

Lemma 18. *Let n and α be integers such that $n \geq 7$ and $2 \leq \alpha \leq n$, then*

$$\frac{f_{\mathsf{T}}(n, \alpha)}{\alpha - 1} \leq \frac{2^n}{n - 1}. \tag{11}$$

Proof. We consider three cases $\alpha = n$, $\alpha = 2$ and $3 \leq \alpha \leq n - 1$. Let $q = n - \left\lceil \frac{n}{\alpha} \right\rceil$ be the order of the graph obtained by removing a clique of maximal size in $\mathsf{T}_{n,\alpha}$.

(*i*) Suppose that $\alpha = n$. In this case, both sides of Ineq. (11) are equal and the result trivially holds.

(*ii*) Suppose that $\alpha = 2$. If n is even, $f_{\mathsf{T}}(n, 2) = \frac{n^2}{4} + n + 1$ and if n is odd, $f_{\mathsf{T}}(n, 2) = \frac{n^2}{4} + n + \frac{3}{4}$. Hence

$$f_{\mathsf{T}}(n, 2)(n - 1) \leq \left(\frac{n^2}{4} + n + 1\right)(n - 1).$$

The latter function is cubic, and thus strictly less than 2^n when $n \geq 7$. The result holds in case $\alpha = 2$.

(*iii*) Suppose now that $3 \leq \alpha \leq n - 1$. The proof will use an induction on n. If $7 \leq n \leq 10$, Ineq. (11) can be checked by easy computation and we assume that $n \geq 11$. By Lemma 6, we have

$$\frac{f_{\mathsf{T}}(n, \alpha)}{\alpha - 1} = \frac{f_{\mathsf{T}}(n - 1, \alpha)}{\alpha - 1} + \frac{f_{\mathsf{T}}(q, \alpha - 1)}{\alpha - 1} \leq \frac{f_{\mathsf{T}}(n - 1, \alpha)}{\alpha - 1} + \frac{f_{\mathsf{T}}(q, \alpha - 1)}{\alpha - 2}.$$

We can use induction for $f_{\mathsf{T}}(n - 1, \alpha)/(\alpha - 1)$ because either we fall in case (*i*) when $\alpha = n - 1$, or we stay in case (*iii*). We can also use induction for $f_{\mathsf{T}}(q, \alpha - 1)/(\alpha - 2)$. Indeed, if $\alpha - 1 = 2$ or $\alpha - 1 = q$, we fall in cases (*ii*) and (*i*), respectively. Otherwise, notice that

$$q = n - \left\lceil \frac{n}{\alpha} \right\rceil > n - \left\lceil \frac{n}{3} \right\rceil \geq n - \frac{n + 2}{3}. \tag{12}$$

16

Hence, $q \geq 7$ when $n \geq 11$, and we fall in case (iii). It follows that

$$\frac{f_{\mathsf{T}}(n,\alpha)}{\alpha - 1} \leq \frac{2^{n-1}}{n-2} + \frac{2^q}{q-1}.$$

As $2^q/(q-1)$ is an increasing function, it is maximum when $q = n - 2$. This leads to

$$\frac{f_{\mathsf{T}}(n,\alpha)}{\alpha - 1} \leq \frac{2^{n-1}}{n-2} + \frac{2^{n-2}}{n-3} \leq \frac{2^{n-1}}{n-3} + \frac{2^{n-2}}{n-3} = \frac{3 \cdot 2^n}{4(n-3)}.$$

To finish the proof, one has to check if

$$\frac{3}{4(n-3)} \leq \frac{1}{n-1}.$$

This is the case when $n \geq 9$. $\qquad\square$

Lemma 19. *Let G be a graph of order $n \geq 5$ with a stability number α and a Fibonacci index F, then*

$$F \leq \frac{2^n - n - 1}{n - 1}(\alpha - 1) + n + 1,$$

with equality if and only if $G \simeq \mathsf{K}_n$ or $G \simeq \overline{\mathsf{K}_n}$.

Proof. Notice that the right hand side of the inequality in this lemma is equal to $\mathsf{L}_n(\alpha)$ (see Figures 3 and 4).

The cases $\alpha = 1$ and $\alpha = n$ are trivial and correspond to both cases of equality with $G \simeq \mathsf{K}_n$ and $G \simeq \overline{\mathsf{K}_n}$, respectively. We now assume that $2 \leq \alpha \leq n - 1$ and we prove the strict inequality $F < \mathsf{L}_n(\alpha)$. By Theorem 8, it suffices to show that $f_{\mathsf{T}}(n,\alpha) < \mathsf{L}_n(\alpha)$. The cases $n = 5$ and $n = 6$ can be easily checked by computation and we suppose that $n \geq 7$.

To achieve this aim, we use the following geometrical argument. For a fixed value of n, we consider two lines. The first one is $y = \mathsf{L}_n(x)$ and the second one is the line passing by the points $(1, n+1)$, $(\alpha, f_{\mathsf{T}}(n,\alpha))$ corresponding to K_n and $\mathsf{T}_{n,\alpha}$, respectively. The first line has slope

$$\frac{2^n - n - 1}{n - 1},$$

and the second line has slope

$$\frac{f_{\mathsf{T}}(n,\alpha) - (n+1)}{\alpha - 1}.$$

We now prove that the slope of the second line is strictly less than the slope if the first line. As $\alpha < n$ and by Lemma 18,

$$\frac{f_{\mathsf{T}}(n,\alpha) - (n+1)}{\alpha - 1} < \frac{f_{\mathsf{T}}(n,\alpha)}{\alpha - 1} - \frac{n+1}{n-1} \leq \frac{2^{n-1}}{n-1} - \frac{n+1}{n-1},$$

and the result holds.

$\qquad\square$

We now consider the class $\mathcal{C}(n)$, and we make the same kind of computations of done in the two previous lemmas, but with respect to the line $y = \mathsf{L}'_n(x)$.

Lemma 20. *Let n and α be integers such that $n \geq 11$ and $2 \leq \alpha \leq n - 4$, then*

$$\frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} \leq \frac{2^{n-1}}{n - 2}. \tag{13}$$

Proof. The proof is similar to the proof of Lemma 18. We consider three cases $\alpha = 2$, $\alpha = n - 4$ and $3 \leq \alpha \leq n - 5$. Let $q = n - \left\lceil \frac{n}{\alpha} \right\rceil$.

(i) Suppose that $\alpha = 2$. Similarly to case (ii) in the proof of Lemma 18, we have that $f_\mathsf{T}(n, 2) \leq \frac{n^2}{4} + n + 1$. Hence

$$f_\mathsf{T}(n, 2)(n - 2) \leq \left(\frac{n^2}{4} + n + 1 \right)(n - 2).$$

The latter function is cubic, and thus strictly less than 2^{n-1} when $n \geq 9$.

(ii) Suppose that $\alpha = n - 4$. In this case, and as $n \geq 11$, the Turán graph $\mathsf{T}_{n,n-4}$ is isomorphic to the disjoint union of four graphs K_2 and $n - 8$ graphs K_1. Hence,

$$\begin{aligned}
\frac{2^{n-1}}{n - 2} - \frac{f_\mathsf{T}(n, n - 4)}{n - 5} &= \frac{2^7 \cdot 2^{n-8}}{n - 2} - \frac{3^4 \cdot 2^{n-8}}{n - 5}, \\
&= \frac{2^{n-8} \left[(2^7 - 3^4)n - (5 \cdot 2^7 - 2 \cdot 3^4) \right]}{(n - 2)(n - 5)}, \\
&= \frac{2^{n-8} \left[47n - 478 \right]}{(n - 2)(n - 5)},
\end{aligned}$$

which is positive when $n \geq 11$. Ineq. (13) holds in this case.

(iii) Suppose now that $3 \leq \alpha \leq n - 5$. We use an induction on n. If $11 \leq n \leq 16$, Ineq. (13) can be checked by computation and we assume that $n \geq 17$. Similarly to case (iii) in the proof of Lemma 18, we have

$$\frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} \leq \frac{f_\mathsf{T}(n - 1, \alpha)}{\alpha - 1} + \frac{f_\mathsf{T}(q, \alpha - 1)}{\alpha - 2},$$

and we can use induction for both terms. Indeed for $f_\mathsf{T}(n - 1, \alpha)/(\alpha - 1)$ we fall in case (ii) when $\alpha = n - 5$, or we stay in case (iii). For $f_\mathsf{T}(q, \alpha - 1)/(\alpha - 2)$, since $3 \leq \alpha \leq n - 5$, we can check that either $\alpha - 1 = 2$ or $\alpha - 1 = q - 4$ two cases already treated in (i) and (ii), or $3 \leq \alpha - 1 \leq q - 5$. In the latter case, we have $q \geq 11$ when $n \geq 17$ by Ineq. (12). It follows that

$$\frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} \leq \frac{2^{n-2}}{n - 3} + \frac{2^{q-1}}{q - 2}.$$

18

As $2^q/(q-2)$ is increasing, it is maximum when $q = n - 2$. This leads to

$$\frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} \leq \frac{2^{n-2}}{n - 3} + \frac{2^{n-3}}{n - 4} \leq \frac{3 \cdot 2^{n-1}}{4(n - 4)}.$$

The proof is completed because

$$\frac{3}{4(n - 4)} \leq \frac{1}{n - 2}$$

when $n \geq 10$. $\qquad\square$

Lemma 21. *Let G be a connected graph of order $n \geq 8$ with a stability number α and a Fibonacci index F, then*

$$F \leq \frac{2^{n-1} - n}{n - 2}(\alpha - 1) + n + 1,$$

with equality if and only if $G \simeq \mathsf{K}_n$ or $G \simeq \mathsf{S}_n$.

Proof. Observe that the right hand side of the inequality stated in the lemma is equal to $\mathsf{L}'_n(\alpha)$ (see Figure 4).

The cases $\alpha = 1$ and $\alpha = n - 1$ are trivial and correspond to the two cases of equality. When $2 \leq \alpha \leq n - 2$, we prove the strict inequality $F < \mathsf{L}'_n(\alpha)$. The cases $n = 8$, $n = 9$ and $n = 10$ can be checked by computation and we therefore suppose that $n \geq 11$. We consider separately the two cases $2 \leq \alpha \leq n - 4$ and $n - 3 \leq \alpha \leq n - 2$.

(i) Let $2 \leq \alpha \leq n - 4$. By Theorem 12, it is enough to show that $f_\mathsf{TC}(n, \alpha) < \mathsf{L}'_n(\alpha)$. We prove a stronger result, that is, $f_\mathsf{T}(n, \alpha) < \mathsf{L}'_n(\alpha)$. The result follows since $f_\mathsf{TC}(n, \alpha) \leq f_\mathsf{T}(n, \alpha)$. This situation is well illustrated in Figure 4 which also indicates that the case $n - 3 \leq \alpha \leq n - 2$ has to be treated separately.

The argument to prove that $f_\mathsf{T}(n, \alpha) < \mathsf{L}'_n(\alpha)$ is the same as in the proof of Lemma 19. We show that the slope of the line $y = \mathsf{L}'_n(x)$ is strictly greater than the slope of the line passing by the two points corresponding to K_n and $\mathsf{T}_{n,\alpha}$.

As $\alpha \leq n - 4$, we have

$$\frac{n + 1}{\alpha - 1} \geq \frac{n + 1}{n - 5} > \frac{n}{n - 2}.$$

This observation and Lemma 20 lead to

$$\frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} - \frac{n + 1}{\alpha - 1} < \frac{f_\mathsf{T}(n, \alpha)}{\alpha - 1} - \frac{n}{n - 2} \leq \frac{2^{n-1}}{n - 2} - \frac{n}{n - 2},$$

and the announced property on the slopes is proved.

19

(ii) Let $n-3 \le \alpha \le n-2$. By Theorem 12, one has to show that $f_{\mathsf{TC}}(n, n-2) < \mathsf{L}'_n(n-2)$ and $f_{\mathsf{TC}}(n, n-3) < \mathsf{L}'_n(n-3)$. It suffices to prove that

$$f_{\mathsf{TC}}(n, n-2) < \mathsf{L}'_n(n-3).$$

Indeed, $f_{\mathsf{TC}}(n, n-3) < f_{\mathsf{TC}}(n, n-2)$ by Corollary 14 and $\mathsf{L}'_n(n-3) < \mathsf{L}'_n(n-2)$ because the slope of $y = \mathsf{L}'_n(x)$ is strictly positive. As $n \ge 11$, we have $\alpha \ge \frac{n}{2}$ and we use Corollary 13 to compute $f_{\mathsf{TC}}(n, n-2)$. This leads to

$$
\begin{aligned}
\mathsf{L}'_n(n-3) - f_{\mathsf{TC}}(n, n-2) \;\; &= \frac{2^{n-1}-n}{n-2}(n-4) + n + 1 - 3 \cdot 2^{n-3} - 2, \\
&= \frac{(n-10) \cdot 2^{n-3} + n + 2}{n-2},
\end{aligned}
$$

which is strictly positive when $n \ge 10$. $\qquad\square$

We can now give the proof of Theorems 15 and 16.

Proof of Theorems 15 and 16. We begin with the proof for the polytope $\mathcal{P}_{\mathcal{G}(n)}$. Looking at Lemma 17, it remains to prove that (i) Ineq. (7) is facet defining; (ii) there are exactly n facet defining inequalities of $\mathcal{P}_{\mathcal{G}(n)}$.

The proof (i) is straightforward. Indeed, Lemma 19 ensures that Ineq. (7) is valid. Moreover, the points $(1, n+1)$ and $(n, 2^n)$ correspond to the graphs K_n and $\overline{\mathsf{K}_n}$, respectively. These points are affinely independent and satisfy Ineq. (7) with equality. Therefore Ineq. (7) is facet defining.

For (ii), it suffices to observe that for any value of $x = 1, 2, \ldots, n$, there is exactly one vertex in the polytope: the point which correspond to the complete split graph $\mathsf{CS}_{n,x}$. It follows that $\mathcal{P}_{\mathcal{G}(n)}$ has exactly n vertices and n facets.

The proof is similar for the polytope $\mathcal{P}_{\mathcal{C}(n)}$ except that $x < n$. Indeed, Ineq. (9) is valid by Lemma 21, and the points satisfying Ineq. (9) with equality correspond to the graphs K_n and S_n. $\qquad\square$

6 Observations

Turán graphs $\mathsf{T}_{n,\alpha}$ have minimum size inside $\mathcal{G}(n, \alpha)$ by the Theorem of Turán [23]. Christophe et al. [6] give a tight lower bound for the connected case of this theorem, and Bougard and Joret [2] characterized the extremal graphs, which happen to contain the $\mathsf{TC}_{n,\alpha}$ graphs as a subclass.

By these results and Theorems 8 and 12, we can observe the following relations between graphs with minimum size and maximum Fibonacci index. The graphs inside $\mathcal{G}(n, \alpha)$ minimizing $m(G)$ are exactly those which maximize $F(G)$. This is also true for the graphs

inside $\mathcal{C}(n,\alpha)$, except that there exist other graphs with minimum size than the Turán-connected graphs.

However, these observations are not a trivial consequence of the fact that $F(G) < F(G^e)$ where e is any edge of a graph G. As indicated in our proofs, the latter property only implies that a graph maximizing $F(G)$ contains only α-critical edges (and α-safe bridges for the connected case). Our proofs use a deep study of the structure of the extremal graphs to obtain Theorems 8 and 12.

We now give additional examples showing that the intuition that more edges imply fewer stable sets is wrong. Pedersen and Vestergaard [19] give the following example. Let r be an integer such that $r \geq 3$, G_1 be the Turán graph $\mathsf{T}_{2r,r}$ and G_2 be the star S_{2r}. The graphs G_1 and G_2 have the same order but G_1 has less edges (r) than G_2 ($2r-1$). Nevertheless, observe that $F(G_1) = 3^r < F(G_2) = 2^{2r-1} + 1$. This example does not take into account the stability number since $\alpha(G_1) = r$ and $\alpha(G_2) = 2r - 1$.

We propose a similar example of pairs of graphs with the same order and the same stability number (see the graphs G_3 and G_4 on Figure 5). These two graphs are inside the class $\mathcal{G}(6,4)$, however $m(G_3) < m(G_4)$ and $F(G_3) < F(G_4)$. Notice that we can get such examples inside $\mathcal{G}(n,\alpha)$ with n arbitrarily large, by considering the union of several disjoint copies of G_3 and G_4.
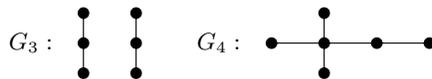

Figure 5: Graphs with same order and stability number

These remarks and our results suggest some questions about the relations between the size, the stability number and the Fibonacci index of graphs. What are the lower and upper bounds for the Fibonacci index inside the class $\mathcal{G}(n,m)$ of graphs order n and size m; or inside the class $\mathcal{G}(n,m,\alpha)$ of graphs order n, size m and stability number α? Are there classes of graphs for which more edges always imply fewer stable sets? We think that these questions deserve to be studied.

Acknowledgments

References

[1] BERGE, C. *The Theory of Graphs*. Dover Publications, New York, 2001.

[2] BOUGARD, N., AND JORET, G. Turán Theorem and k-connected graphs. *J. Graph Theory 58* (2008), 1 – 13.

[3] BROOKS, R.-L. On colouring the nodes of a network. *Proc. Cambridge Philos. Soc. 37* (1941), 194 – 197.

[4] BRUYÈRE, V., AND MÉLOT, H. Turàn Graphs, Stability Number, and Fibonacci Index. In *Combinatorial Optimization and Applications, COCOA 2008* (St. John's, Newfoundland, Canada, 2008), vol. 5165 of *Lecture Notes in Computer Science*, Springer–Verlag, pp. 127 – 138.

[5] BYSKOV, J.M. Enumerating maximal independent sets with applications to graph colouring. *Oper. Res. Lett. 32* (2004), 547 – 556.

[6] CHRISTOPHE, J., DEWEZ, S., DOIGNON, J.-P., ELLOUMI, S., FASBENDER, G., GRÉGOIRE, P., HUYGENS, D., LABBÉ, M., MÉLOT, H., AND YAMAN, H. Linear inequalities among graph invariants: using GraPHedron to uncover optimal relationships. Accepted for publication in *Networks* (2008), 24 pages.

[7] ERDÖS, P., AND GALLAI, T. On the minimal number of vertices representing the edges of a graph. *Magyar Tud. Akad. Mat. Kutató Int. Közl. 6* (1961), 181–203.

[8] GRAPHEDRON. Reports on the study of the Fibonacci index and the stability number of graphs and connected graphs. URL: `www.graphedron.net/index.php?page=viewBib&bib=10`.

[9] GUTMAN, I., AND POLANSKY, O.E. *Mathematical Concepts in Organic Chemistry*. Springer-Verlag, Berlin, 1986.

[10] HEUBERGER, C., AND WAGNER, S. Maximizing the number of independent subsets over trees with bounded degree. *J. Graph Theory 58* (2008), 49 – 68.

[11] JORET, G. *Entropy and Stability in Graphs*. PhD thesis, Université Libre de Bruxelles, Belgium, 2007.

[12] KNOPFMACHER, A., TICHY, R.F.., WAGNER, S., AND ZIEGLER, V. Graphs, partitions and Fibonacci numbers. *Discrete Appl. Math. 155* (2007), 1175 – 1187.

[13] LI, X., LI, Z., AND WANG, L. The Inverse Problems for Some Topological Indices in Combinatorial Chemistry. *J. Comput. Biol. 10*, 1 (2003), 47 – 55.

[14] LI, X., ZHAO, H., AND GUTMAN, I. On the Merrifield-Simmons Index of Trees. *MATCH Comm. Math. Comp. Chem. 54* (2005), 389 – 402.

[15] LOVÁSZ, L., AND PLUMMER, M.D. *Matching Theory*. Akadémiai Kiadó - North-Holland, Budapest, 1986.

[16] MÉLOT, H. Facet Defining Inequalities among Graph Invariants: the system GraPHedron. *Discrete Applied Mathematics 156* (2008), 1875–1891.

[17] MERRIFIELD, R.E.., AND SIMMONS, H.E.. *Topological Methods in Chemistry*. Wiley, New York, 1989.

[18] PEDERSEN, A.S., AND VESTERGAARD, P.D. The number of independent sets in unicyclic graphs. *Discrete Appl. Math. 152* (2005), 246 – 256.

[19] PEDERSEN, A.S., AND VESTERGAARD, P.D. Bounds on the Number of Vertex Independent Sets in a Graph. *Taiwanese J. Math. 10*, 6 (2006), 1575 – 1587.

[20] PEDERSEN, A.S., AND VESTERGAARD, P.D. An Upper Bound on the Number of Independent Sets in a Tree. *Ars Combin. 84* (2007), 85 – 96.

[21] PRODINGER, H., AND TICHY, R.F.. Fibonacci numbers of graphs. *Fibonacci Quart. 20*, 1 (1982), 16 – 21.

[22] TICHY, R.F., AND WAGNER, S. Extremal Problems for Topological Indices in Combinatorial Chemistry. *J. Comput. Biol. 12*, 7 (2005), 1004 – 1013.

[23] TURÁN, P. Eine Extremalaufgabe aus der Graphentheorie. *Mat. Fiz. Lapok 48* (1941), 436–452.

[24] WAGNER, S. Extremal trees with respect to Hosoya Index and Merrifield-Simmons Index. *MATCH Comm. Math. Comp. Chem. 57* (2007), 221 – 233.

[25] WANG, H., AND HUA, H. Unicycle graphs with extremal Merrifield-Simmons Index. *J. Math. Chem. 43*, 1 (2008), 202 – 209.

[26] WANG, M., HUA, H., AND WANG, D. The first and second largest Merrifield-Simmons indices of trees with prescribed pendent vertices. *J. Math. Chem. 43*, 2 (2008), 727 – 736.