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Problems article

Graphs whose vertices are forests with bounded degree: Open problems

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Abstract A graph G is said to be an f-*graph* if G has no vertex of degree greater than f. Define $F(n, f)$ to be the graph with vertices the set of unlabeled f-forests of order n with vertex v adjacent to vertex u if and only if v and u differ by exactly one edge. Note that if v is adjacent to u, then either v is a one-edge deleted sub f-forest of u or v is a one-edge extended super f-forest of u. A number of papers investigating these graphs have recently appeared. Here a set is compiled of open problems concerning various parameters for these graphs. Specifically, problems associated with order, size, traceability, planarity, diameter, domination, and applications in chemistry are presented.

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1 Introduction

A graph G is said to be an f*-graph* if G has no vertex of degree greater than f. Define $F(n,f)$ to be the graph with vertices the set of unlabeled f-forests of order n with vertex v adjacent to vertex u if and only if v and u differ by exactly one edge. Note that if v is adjacent to u, then either v is a one-edge deleted sub f-forest of u or v is a one-edge extended super f-forest of u. A number of papers investigating these graphs have recently appeared and are noted in the references. These investigations have given rise to a number of open problems concerning various parameters for these graphs. In particular, problems associated with order, size, traceability, planarity, diameter, domination, and applications in chemistry are presented.

2 Order

There are algorithms for computing the order of $F(n,f)$, (see [3, 9]). Thus it is of interest to find improvements of these algorithms. It is also of interest to find other interpretations of the sequence of the orders of $F(n,f)$ for different values of f. For example, the order of $F(n,2)$ is precisely the number of unrestricted partitions of n [9] whose initial values are listed as the sequence A000041 in [14].

Problem 2.1 *Are there other interpretations of the sequence of orders of* $F(n,f)$ *for* $f \geq 2$*?*

Problem 2.2 *Is it possible to find and/or reasonable to ask about generating function formulations for the order of* $F(n,f)$*?*

3 Size

As with the order of $F(n,f)$ there are algorithms for computing the size of $F(n,f)$ [9]. Similarly, as for order:

Problem 3.1 *Are there other interpretations of the sequence of the sizes of* $F(n,f)$ *for* $f \geq 2$*?*

Problem 3.2 *Is it possible to find and/or reasonable to ask about generating function formulations for the size of* $F(n,f)$*?*

The ratio of the size to the order of $F(n,f)$ is defined to be the *edge density* of $F(n,f)$, see [6].

Problem 3.3 *Determine whether for all* $n \geq 5$ *the edge density of* $F(n,f)$ *is unimodal with respect to increasing* f *with maximum value at some* $f < n-1$.

Problem 3.4 *For a given n determine the value of f at which the edge density is maximum.*

For a connected graph G, the relation $|E(G)| - |V(G)| + 1$ equals the number of independent cycles in G. This is known as the *Betti number of* G, denoted $\beta(G)$. Thus, the results on order and size of $F(n, f)$ yield the *Betti number of* $F(n, f)$, which in turn provides information about other properties of $F(n, f)$.

Problem 3.5 *Investigate various cycle properties of $F(n, f)$. For example, determine the circumference of $F(n, f)$ (see Section 4).*

4 Traceability

Since $F(n, f)$ for $n \geq 4$ always has a pendant vertex and at most two pendant vertices, the latter occurring if and only if $f = 1$ or $n-1$ (see Theorem 2.4 [10]), $F(n, f)$ never has a *Hamilton cycle*, that is, a cycle that contains every vertex. However, $F(n, f)$ may contain a path that contains every vertex, namely, a *Hamilton path*. Such a graph is called *traceable*. The traceability properties of $F(n, f)$ have been studied in [10, 12].

Problem 4.1 *Prove the conjecture [10] that $F(n, f)$ is non-traceable for $n \geq 10$ and $3 \leq f \leq n-1$.*

Let $F^*(n, f)$ denote $F(n, f)$ with its pendant vertices deleted.

Problem 4.2 *Does $F^*(n, f)$ contain a Hamilton cycle?*

Note that if $F^*(n, f)$ contains a Hamilton cycle, then in the cases where $F(n, f)$ had a single pendant vertex, $F(n, f)$ will be traceable.

5 Planarity

The question of the planarity of $F(n, f)$ is completely solved via the following theorem.

Theorem 5.1 (Theorem 2.1 in [6])

(a) $F(n, f)$ *is nonplanar for all* n, f *such that* $n \geq 6$ *and* $3 \leq f \leq n-1$.

(b) $F(n, f)$ *is planar for all* n, f *such that* $1 \leq n \leq 5$ *and* $0 \leq f \leq n-1$.

(c) $F(n, 2)$ *is nonplanar for all* $n \geq 7$ *and planar for all* $3 \leq n \leq 6$.

(d) $F(n, f)$ *is planar for* $f = 0$, $n \geq 1$ *and* $f = 1$, $n \geq 2$.

Problem 5.1 *For the nonplanar cases, what is the genus of $F(n, f)$?*

Theorem 5.1 yields all $F(n, f)$ with genus $\gamma(F(n, f))$ at least 1. There are some basic theorems that provide results concerning the lower bound for the genus $\gamma(G)$ of a graph G. An example is the following.

Theorem 5.2 (Theorem 15.4.1, p. 526 in [11]) *If G is connected, then*

$$\gamma(G) \geq \left\lceil \frac{|E(G)|(\mathrm{girth}(G)-2)}{2\,\mathrm{girth}(G)} - |V(G)| + 1 \right\rceil.$$

Since $F(n, f)$ is bipartite and has girth 4 for all $n \geq 4$ and $2 \leq f \leq n-1$, the next corollary follows directly.

Corollary 5.2.1 *If $n \geq 4$ and $2 \leq f \leq n-1$, then*

$$\gamma(F(n, f)) \geq \left\lceil \frac{|E(F(n, f))|}{4} - \frac{|V(F(n, f))|}{2} + 1 \right\rceil.$$

Applying the result $|E(F(8,2))| = 47$ and $|V(F(8,2))| = 22$ (see [3]) it follows that $\gamma(F(8,2)) \geq 2$. Similar results follow from the known sizes of various $F(n, f)$ (see [3]).

6 Diameter

The *distance* $d(G,H)$ between two vertices G and H in $F(n, f)$ is defined as the least number of insertions and deletions in G to obtain H. This is equivalent to the standard definition of graph distance in $F(n, f)$. A basic result for the insertion/deletion definition for the distance between G and H is

$$d(G,H) = |E(G)| + |E(H)| - 2|E(I)|,$$

where I is the largest size common subgraph of G and H. This played a central role in the determination of the next theorem.

Theorem 6.1 (Theorems 2.5 and 3.1 in [13])

(a) diam $F(n,0) = 0$, diam $F(n,1) = \lfloor n/2 \rfloor$, diam $F(n,2) =$ diam $F(n,3) = n-1$.

(b) If $4 \leq f \leq n-3$ with fixed f and $n \to \infty$, then

$$\frac{2f-3}{f+1} n(1+o(1)) \leq \mathrm{diam}\, F(n, f) \leq 2n(1+o(1)).$$

(c) diam $F(n, n-2) = 2n-7$ *for $n \geq 6$, and* diam $F(n, n-1) = 2n-6$ *for $n \geq 5$.*

Problem 6.1 *What is* diam $F(n, f)$ *for $4 \leq f \leq n-3$?*

Of particular interest, is the case $f = 4$, because of its relation to chemistry (see Section 8 and [4, 7, 8]).

7 Domination

In [3] algorithms for computing the domination number of $F(n,f)$ are presented together with the investigation of various domination properties of $F(n,f)$.

Problem 7.1 *Obtain asymptotic properties of the domination number of $F(n,f)$.*

Consider $\deg_{\text{av}}(F(n,f)) = 2|E(F(n,f))|/|V(F(n,f))|$, the *average (mean)* vertex degree of $F(n,f)$, and $\Delta(F(n,f))$, the *maximum* degree of a vertex in $F(n,f)$. Note that $\deg_{\text{av}}(F(n,f))$ is twice the edge density (see Section 3), and that $\Delta(F(n,f))$ plays a role in domination studies [3].

Problem 7.2 *Is there a meaningful relation between $\deg_{\text{av}}(F(n,f))$ or $\Delta(F(n,f))$ and the domination number of $F(n,f)$?*

8 Applications in Chemistry

A relation of $F(n,4)$ to an application in chemistry was investigated in [4, 5, 7, 8].

First note that the 4-trees of order n are in a one-to-one correspondence with the saturated hydrocarbons with n carbons, also called *alkanes*, that is, the molecules with structural formula C_nH_{2n+2}. This is so because the carbon skeleton of these molecules has the same structure as a 4-tree of order n. For a detailed and historical overview of this correspondence see pp. 2–4 in [1]. Next note that a vertex of $F(n,4)$, being a forest of 4-trees whose orders add up to n, can be conveniently interpreted as a mixture of alkanes. The graph $F(n,4)$ can be thought of as having its vertex set all possible alkane mixtures with representative an n-carbon alkane mixture. Adjacency is interpreted as the breaking or creating of chemical bonds. A tie in with current research in chemistry concerns the conversion of methane to higher alkanes. This is explored in [4, 5] using $F(n,4)$ as a model.

Problem 8.1 *Find other chemistry results in converting methane to higher alkanes. Use these results to extend the $F(n,4)$ model for both descriptive and extrapolation purposes.*

Problem 8.2 *Find the value of n that is optimum for describing physical results via the $F(n,4)$ model as was done in [4, 5]. Note that small n may be too coarse and that large n beyond some specified value may provide only negligible additional insight.*

9 Concluding remarks

Graphs whose vertices are graphs (in general) with bounded degree have a rich history of research and open problems [2]. Here the focus is on graphs that are forests with bounded degree and it has been shown that with just this restriction many open problems exist.

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