HAMILTON PATHS IN GRAPHS WHOSE VERTICES ARE GRAPHS

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Abstract: Let $U(n, f)$ denote the graph with vertex set the set of unlabeled graphs of order n that have no vertex of degree greater than f. Two vertices H and G of $U(n, f)$ are adjacent if and only if H and G differ (up to isomorphism) by exactly one edge. The problem of determining the values of n and f for which $U(n, f)$ contains a Hamilton path is investigated. There are only a few known non-trivial cases for which a Hamilton path exists. Specifically, these are $U(5, 3)$, $U(6, 3)$, and $U(7, 3)$. On the other hand there are many cases for which it is shown that no Hamilton path exists. The complete solution of this problem is unresolved.

1. Introduction

By an f-graph we mean a graph having no vertex of degree greater than f. Let $U(n, f)$ denote the graph whose vertex set consists of all unlabeled f-graphs of order $n \geq f + 1$. A pair $\{G, H\}$ of f-graphs of order n is an edge in $U(n, f)$ if and only if G and H differ (up to isomorphism) by exactly one edge.

The graph $U(n, f)$ is the underlying graph of $D(n, f)$, the transition digraph for the Random f-Graph Process [1] and any Markov process whose states are the unlabelled f-graphs of order n such that all of its transitions are one-edge extensions with non-zero probability, for example see [2][3]. Such processes are prototypes for random graph process having a variety of applications, for example, see [4]. The transition digraphs $D(4, 2)$ and $D(4, 3)$ are shown in Figures 1 and 2, respectively.

At each step of this process exactly one edge is added, thus $U(n, f)$ is bipartite with its vertices that correspond to even and odd size graphs forming a bipartite vertex set partition.

An f-graph G is *edge-maximal* (EM f-graph), if no edge can be added to it without introducing a vertex of degree greater than f. The f-graph G is *edge-transitive* (ET f-graph), if for each pair of edges e_1 and e_2 in G, there is an automorphism of G that sends e_1 to e_2. We call an f-graph that is both EM and ET an EMT f-graph. A vertex of degree one in $U(n, f)$ is a *pendant vertex*. The following is obvious:

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(i) An EM f-graph does not have any f-graph one-edge-extended supergraphs.

(ii) An ET f-graph, other than K_n^c, the *empty graph*, has a unique proper one-edge-deleted subgraph.

(iii) An EMT f-graph corresponds to a pendant vertex $U(n, f)$.

Let P_k denote a *path of order k*. If we wish to specify the starting and ending vertices of a path from x to y, we write $x \rightarrow y$. The latter is defined as a sequence x_1, $x_2, \ldots, x_k$ of distinct vertices of $U(n, f)$ such that $x_1 = x$, $x_k = y$, and $\{x_i, x_{i+1}\}$ is an edge of $U(n, f)$ for each $i = 1, 2, \ldots, k-1$. Let $N(n, f)$ denote the *order of* $U(n, f)$. A *Hamilton path* in $U(n, f)$ is a path with $k = N(n, f)$.

General Problem. Determine the values of n and f for which $U(n, f)$ contains a Hamilton path.

The cases $U(n,0) \cong K_1, U(n,1) \cong P_{\lceil (n+1)/2 \rceil}$, and $U(3,2) \cong P_4$ being paths, each contain a Hamilton path, but are considered trivial.

For $f = 2$, and $n \geq 4$, no $U(n, 2)$ has a Hamilton path. This follows easily from observations that are made in Section 2 (see Theorem 2.5). In Section 3 we consider $f = n - 1$ and state the first open problem. The case $f = 3$ is considered in Section 4 and where the only known nontrivial examples, for any f, having a Hamilton path are given. Namely, $U(5, 3)$, $U(6, 3)$, and $U(7, 3)$. It is noted that some of the methods used when $f = 3$ apply when $f \geq 4$. However, other than for $f = 0$, 1, and 2, the complete solution of the General Problem remains unresolved.

2. Basic observations and $f = 2$ with $n > 3$

$U(n, f)$ is a connected graph and it is obvious that, if $U(n, f)$ has more than two pendant vertices, then $U(n, f)$ does not contain a Hamilton path. When $f = n - 1$, $U(n, f)$ always has exactly two pendant vertices, namely, the vertices associated with K_n^c and K_n. However, when $f < n - 1$ there are cases when $U(n, f)$ will have at least three pendant vertices. Such cases provide a sufficient condition for the nonexistence of a Hamilton path in $U(n, f)$.

Our first lemma provides necessary conditions for the existence of a Hamilton path.

Let $e_f(n)$ and $o_f(n)$ denote the number of unlabeled f-graphs of *order n having even and odd size*, respectively.

Lemma 2.1. If $U(n, f)$ contains a Hamiliton path $K_n^c \rightarrow G$, then

(a) The order $N(n, f)$ of $U(n, f)$ and the size of G have opposite parity.

(b) $e_f(n) - o_f(n) = 0$ when $N(n, f)$ is even ; $e_f(n) - o_f(n) = 1$ when $N(n, f)$ is odd.

(c) $U(n, f)$ has no more than two pendant vertices.

Proof. (a) Since K_n^c is a pendant vertex in $U(n,f)$, every Hamilton path in $U(n,f)$ must have K_n^c as one of its endvertices. Let $K_n^c \to G$ be a Hamilton path in $U(n,f)$. Then, since $U(n,f)$ is bipartite, $|e_f(n) - o_f(n)| \leq 1$. K_n^c has even size, thus, if $N(n,f)$ is even, then $e_f(n) = o_f(n)$ and G must have odd size. Similarly, if $N(n,f)$ is odd, then $e_f(n) = o_f(n) + 1$ and G must have even size.

(b) See proof of (a) and Tables 1 and 2 for data concerning $f = 2$ and 3.

(c) This is a necessary condition for any graph with a Hamilton path. ■

Lemma 2.2. *If there exist two EMT f-graphs G* and *H of order n, then U(n, f) does not contain a Hamilton path and if in addition G* and *H* are *f-regular then U(n + 1, f) does not contain a Hamilton path.*

Proof. By (i), an EM f-graph does not have any one-edge-extended supergraphs that are f-graphs. By (ii), every ET f-graph, other than K_n^c, has the property that, up to isomorphism, it has exactly one one-edge-deleted subgraph. Therefore, the EMT f-graphs G and H each are pendant vertices in $U(n, f)$. Combining this with the fact that K_n^c, which corresponds to a pendant vertex in $U(n, f)$ for all n and f, yields a third pendant vertex in $U(n, f)$. Consequently, $U(n, f)$ cannot contain a Hamilton path.

Note that if in addition G and H are *f-regular*, then $G \cup K_1$ and $H \cup K_1$ are two EMT f-graphs of order $n + 1$. Thus, by the same reasoning as the preceding, $U(n + 1, f)$ does not contain a Hamilton path. ■

Lemma 2.3. *If there exists an EMT f-graph G of order n and an EMT f-graph H of order n - 1, such that $H \cup K_1$ is an EMT f-graph and $G \neq H \cup K_1$, then U(n, f) does not contain a Hamilton path.*

Proof. Since G and $H \cup K_1$ are two nonisomorphic EMT f-graphs of order n, we have by Lemma 2.2, $U(n, f)$ does not contain a Hamilton path. ■

Lemma 2.4. *If n = ab such that there exists EMT f-graphs G_a and G_b of order a and b respectively, then U(n, f) does not contain a Hamilton path and in addition if G_a and G_b are f-regular then U(n+1, f) does not contain a Hamilton path.*

Proof. The graphs aG_b and bG_a (a copies of G_b and b copies of G_a) are distinct EMT f-graphs of order n. Thus, by Lemma 2.2, neither $U(n, f)$ nor $U(n+1, f)$ contain a Hamilton path. ■

Theorem 2.5. *For all $n \geq 4$, U(n, 2) does not contain a Hamilton path.*

Proof. For $n \geq 4$ the n-cycle C_n is an EMT 2-graph of order n and C_{n-1} is an EMT 2-graph of order $n - 1$. Since $C_n \neq C_{n-1} \cup K_1$, we have by Lemma 2.3, $U(n, 2)$ does not contain a Hamilton path. ■

3. $f = n - 1$

As noted in Section 2, $U(1, 0)$, $U(2, 1)$, and $U(3, 2)$ each contain a Hamilton path and are considered trivial for this study. In [5], B.R. Santos showed that $U(4, 3)$ and $U(5, 4)$, which have order 11 and 34, respectively, do not contain a Hamilton path. The following general result by F. Schmidt was also shown in [5]. The proof uses results that are informative and useful in other contexts. Thus, we include it here.

Theorem 3.1. *If* $n \equiv 0,1 \pmod 4$ *and* $n \geq 4$, *then* $U(n, n-1)$ *does not contain a Hamilton path.*

Proof. It was shown by F. Schmidt that, if $U(4, 3)$ has a Hamilton path, then this path must contain the only two edges incident to a pendant vertex in $U(4, 3)$ and every edge that is incident to a vertex of degree 2. This selects 10 such edges and since $U(4, 3)$ has order 11, these must be all of the edges of this Hamilton path. However, these 10 edges do not form a Hamilton path. Thus, $U(4, 3)$ does not contain a Hamilton path.

Assume $n \geq 5$ and $n \equiv 0,1 \pmod 4$. A Hamilton path in the graph $U(n, n-1)$ must alternate between graphs of even size and graphs of odd size. This requires that $| e_{n-1}(n) - o_{n-1}(n) | \leq 1$. In the solution given in [6], it is noted that $e(n) - o(n) = s(n)$, where $s(n)$ is the number of unlabeled self-complementary graphs of order n. Thus, $s(n) \leq 1$. However, this contradicts a known result (see for example, M. Kropar and R.C. Read [7]), that if $n \geq 5$ and $n \equiv 0,1 \pmod 4$, then $s(n) \geq 2$. Thus, $U(n, n-1)$ does not contain a Hamilton path. ■

PROBLEM 1. For what values of $n \equiv 2,3 \pmod 4$ and $n \geq 6$ does $U(n, n-1)$ contain a Hamilton path?

4. $f = 3$

From Theorem 3.1, we have $U(4, 3)$ does not contain a Hamilton path.

The following two algorithms RandHP and ConstrHP have been used to search for Hamilton paths in $U(n, f)$ (see [8]).

Algorithm RandHP

Input: N =order of $U = U(n,f)$; A = adjacency matrix of U; v_1 = pendant vertex in U.

Output: $P = (P_i)$, $1 \leq i \leq N$, a Hamilton path in U, if such a path exists.

Method: A modified DFS method is used. Let X denote the set of visited vertices of the graph U and i be the level of recursion (the number of vertices of a path P).

Step A. Initialization: $X := \varnothing$ and $P_i := 0$ for each $1 \leq i \leq N$.

Step B. Perform the following recursive procedure *HP* with parameters N, $i = 1$, $v = v_1$, A, X, and P.

procedure $HP(N, i, v, A, X, P)$
1. Add vertex v to the path P: $P_i := v$.

2. If $i = N$, then the result is positive; otherwise do the following steps.
   a. Add v to the set X.
   b. Generate σ, a random permutation of $\{1, ..., N\}$.
   c. If for some $j \in \{1, ..., N\}$, $w = \sigma(j) \notin X$, $\{v, w\}$ is an edge in U and $HP(N, i + 1, w, A, X, P)$ is true, then the result is positive; otherwise it is negative.
   d. Remove v from the set X.

ConstrHP
Input: N = the order of U, $A(U)$ = the adjacency matrix of U.

Output: If successful, a Hamilton path in U is obtained.

Method: Initially, let all vertices of U be colored red. If a vertex is assigned to P, then it is recolored green. The number of red neighbors of a vertex is called its *active degree*. A path is constructed starting from both ends, that is, from two pendant vertices x and y of U, both colored green.
At each step i a new vertex is added to P, selected from the neighbors of the previous vertex having *minimum* active degree.
Construction of P from a given end-vertex is continued until conditions for this continuation are not worse than for the other end-vertex.

Theorem 4.1. $U(5, 3)$, $U(6, 3)$, and $U(7, 3)$, *each contain a Hamilton path.*

Proof. $U(5, 3)$ has order 23 (see Table 2), size 46, and exactly two pendant vertices, namely, K_5^c and $K_4 \cup K_1$. An examination of $U(5, 3)$ reveals a Hamilton path (see Figures 3 and 4).

$U(6, 3)$ has order 62 (see Table 2), size 168 and exactly two pendant vertices, namely K_6^c and $K_{3,3}$. The graph $U(7, 3)$ has order 150 and size 562 with pendant vertices K_7^c and $K_{3,3} \cup K_1$. Applying the above algorithms to $U(6, 3)$ and $U(7, 3)$ yields Hamilton paths in these graphs. Due to the order and size of $U(6, 3)$ and $U(7, 3)$, drawings of these graphs and their respective Hamilton paths are not informative and are thereby not given here. ■

A graph G is *totally traceable* means each edge in G is contained in some Hamilton path. Since $U(n, 0)$, $U(n, 1)$, and $U(3, 2)$ are paths, these are trivially totally traceable.

Theorem 4.2. $U(5, 3)$ *is totally traceable.*

Proof. Application of Algorithm RandHP yields at least 971 distinct Hamilton paths in $U(5, 3)$ (see [8]). It is also determined that six of these Hamilton paths is sufficient to cover all of the edges of $U(5, 3)$. ■

PROBLEM 2. For what values of n and f is $U(n,f)$ totally traceable?

A graph G is *vertex-transitive*, if for each pair of vertices x and y, there is an automorphism of G that sends x to y. A graph is called *symmetric*, if it is both edge-transitive and vertex-transitive.

Using the extensive, but not complete, known information on symmetric graphs, one may determine many values of n for which $U(n, 3)$ does not contain a Hamilton path (see Theorem 4.3). The Foster collection of connected symmetric 3-graphs (necessarily 3-regular) (cf. [9]) and its extension by G. Royle, M.D.E. Conder, B. Mckay, and P. Dobscanyi can be accessed at [10]. This web-site lists the known connected symmetric graphs with less than 1,000 vertices. It is known to be complete for up to 768 vertices, but for 770-998 vertices it includes only the Cayley graphs. In [9], the graphs where there is more than one such graph of a given order the order is followed by a capital Latin letter to distinguish these graphs. For example, the existence of the symmetric graph of order 18 and the two symmetric graphs of order 20, is indicated by the listing as 18, 20A, and 20B, respectively. In what follows we denote these graphs F_{18}, F_{20A}, and F_{20B}. For convenience, this extended Foster Census is reproduced here as Table 3.

Theorem 4.3. *For* $n \geq 8$, *the graph* $U(n, 3)$ *does not have a Hamilton path for the following values*:

$n = 10, 11, 14, 15$, and when $n \equiv 0,1 \pmod{x}$,
where $x =$ 8, 12, 18, 20, 28, 30, 42, 50, 52, 70, 76, 78, 98, 102, 110, 114, 124, 130, 148, 172, 182, 186, 190, 222, 244, 258, 266, 268, 292, 310, 316, 338, 366, 370, 388, 402, 412, 430, 434, 436, 438, 474, 484, 494, 506, 508, 518, 556, 582, 602, 604, 610, 618, 628, 652, 654, 670, 722, 724, 726, 730, 762, 772, 790, 796, 806, 834, 844, 854, 892, 906, 916, 938, 942, 962, 964, or 970.

Proof. The cases $n = 4, 5, 6$, and 7 are covered by Theorems 3.1 and 4.1.

For $n = 10, 11, 14$, and 15, the nonexistence of a Hamilton path in $U(n, 3)$ is obtained as follows.

From Table 2 we have the $N(10, 3) = 3{,}547$ and the only possible endvertices of a Hamilton path in $U(10, 3)$, if it exists, are K_{10}^c and P, the Petersen graph. Since P has size 15 we apply the contrapositive of Lemma 2.1(a) to obtain $U(10, 3)$ does not contain a Hamilton path.

If there is a value of n for which $|e_3(n) - o_3(n)| \geq 2$, then applying Lemma 2.1(b)

shows $U(n, 3)$ does not have a Hamilton path. This occurs when $n = 11, 14$, and 15. Here $e_3(11) = 5474$ and $o_3(11) = 5472$ (see Table 2). When $n = 14$, we have

$e_3(14) = 224{,}659$ and $o_3(14) = 224{,}580$. This yields $|e_3(14) - o_3(14)| = 79$ and for $n = 15$, $e_3(15) = 840{,}340$ and $o_3(15) = 840{,}630$, we have $|e_3(15) - o_3(15)| = 290$. Thus, $U(11, 3)$, $U(14, 3)$, and $U(15, 3)$ do not contain a Hamilton path.

To obtain values of $n \geq 8$ and $\neq 10, 11, 14,$ and 15 for which neither $U(n, 3)$ nor $U(n+1, 3)$ contain a Hamilton path, it is sufficient to find pairs, G_1, G_2 of nonisomorphic EMT 3-graphs of order n and apply Lemma 2.2 or pairs G_a, G_b with $n = ab$ and apply Lemma 2.4. Keeping in mind that the graphs in the Foster Census are connected and 3-regular, pairs G_1, G_2 can be obtained by using multiples of these graphs. Note that, for n = 4, 6, 8, and 10, we have the familiar graphs $F_4 = K_4$, $F_6 = K_{3,3}$, $F_8 = Q_3$, the 3-cube, and $F_{10} = P$.

For $n = 8k$, $G_1 = 2kK_4$ and $G_2 = kQ_3$ provide a pair that show the graphs $U(8k, 3)$ and $U(8k + 1, 3)$ do not have a Hamilton path. By completely analogous methods using the graphs in the extended Foster Census it is easily shown that the graphs $U(xk, 3)$ and $U(xk + 1, 3)$, for x as listed in the statement of the theorem, do not have a Hamilton path. In particular, note that if x is on the list given in the statement of the theorem, then no multiple of x need be included on the list. ■

Remark 1. Theorems 3.1, 4.1, and 4.3 cover the cases $n = 4$ up to $n = 21$. Thus, for $f = 3$, the smallest unresolved case of the General Problem is $n = 22$.

PROBLEM 3. Prove or disprove that $U(5, 3)$, $U(6, 3)$ and $U(7, 3)$ are the only nontrivial cases of a $U(n, 3)$ that contains a Hamilton path.

As noted the nontrivial components of the graphs G_1, G_2 used in the proof of Theorem 4.3 were all symmetric graphs, that is, both edge- and vertex-transitive. Therefore, if there exists an EMT, but not vertex-transitive 3-graph of order n, then as above, such a graph can be paired with another of its type or paired with an EMT 3-graph to show the nonexistence of a Hamilton path in $U(n, 3)$.

The Gray graph of order 54 is the smallest order 3-regular edge- but not vertex-transitive graph [11][12]. This graph paired with $9K_{3,3}$ yields $U(54, 3)$ does not have a Hamilton path. However, this result is already contained in Theorem 4.3 by pairing $9K_{3,3}$ with $3F_{18}$ or with the connected symmetric graph F_{54} (see Table 3).

A preprint of paper [13] contains a list of all 3-regular edge- but not vertex-transitive graphs having orders up to 768. Such graphs are called *semisymmetric*. Each of these is an EMT 3-graph. However, each graph in this set that might have been used to obtain a new case of a $U(n, 3)$ with no Hamilton path is already covered by Theorem 4.3. On the other hand, the use of both symmetric and semisymmetric can be applied to obtain a lower bound on the number of pendant vertices in $U(n, 3)$. Specifically, let $B(n)$ denote the number of pendant vertices in $U(n, f)$ and α the number of f-regular graphs of order n that are either symmetric or semisymmetric, then these graphs are EMT f-graphs and by (iii) in Section 1, are pendant vertices in $U(n, f)$. Since K_n^c is always a pendant vertex, $B(n) \geq \alpha + 1$.

PROBLEM 4. Does there exist an f-graph G that corresponds to a pendant vertex in $U(n, f)$ such that G is neither symmetric nor semisymmetric?

5. A comment on forbidden subgraphs

If G is a vertex of degree 2 in $U(n, f)$ and $U(n, f)$ does not contain a Hamilton path that has G as an end vertex, then every Hamilton path in $U(n, f)$ contains the two edges incident to G. This observation leads to noting that:

If $U(n, f)$ has an induced 4-cycle C with a pair of nonadjacent vertices of degree 2 in $U(n, f)$ neither of which are endvertices of a Hamilton path, then every Hamilton path in $U(n, f)$ contains C. Thus, $U(n, f)$ does not contain a Hamilton path.

The graph $U(4, 3)$ contains a 4-cycle of type C (see Figures 2 and 4).

PROBLEM 5. Find subgraphs X of $U(n, f)$ such that if $U(n, f)$ contains X in some designated form, then $U(n, f)$ does not contain a Hamilton path.

Acknowledgements

Partial support of this work was provided in part by research and travel grants from The Technical University of Poznań, The School of Computer Science and Information Systems, Pace University, New York, and The Dyson College of Arts and Sciences, Pace University, New York.

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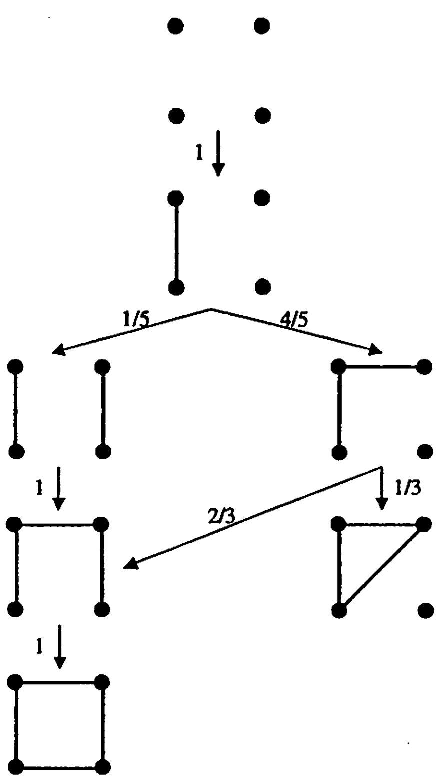


Figure 1. The transition digraph $D(4, 2)$

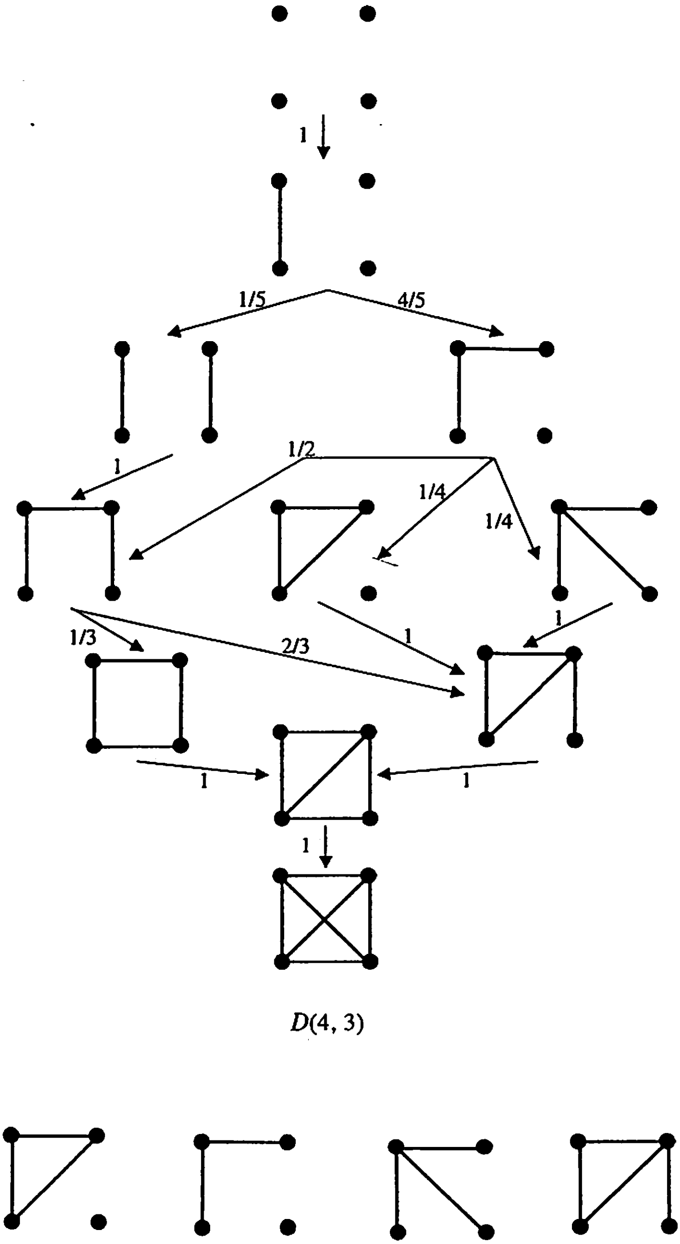


Figure 2. The transition digraph $D(4, 3)$ and the four graphs that induce a 4-cycle in the graph $U(4, 3)$

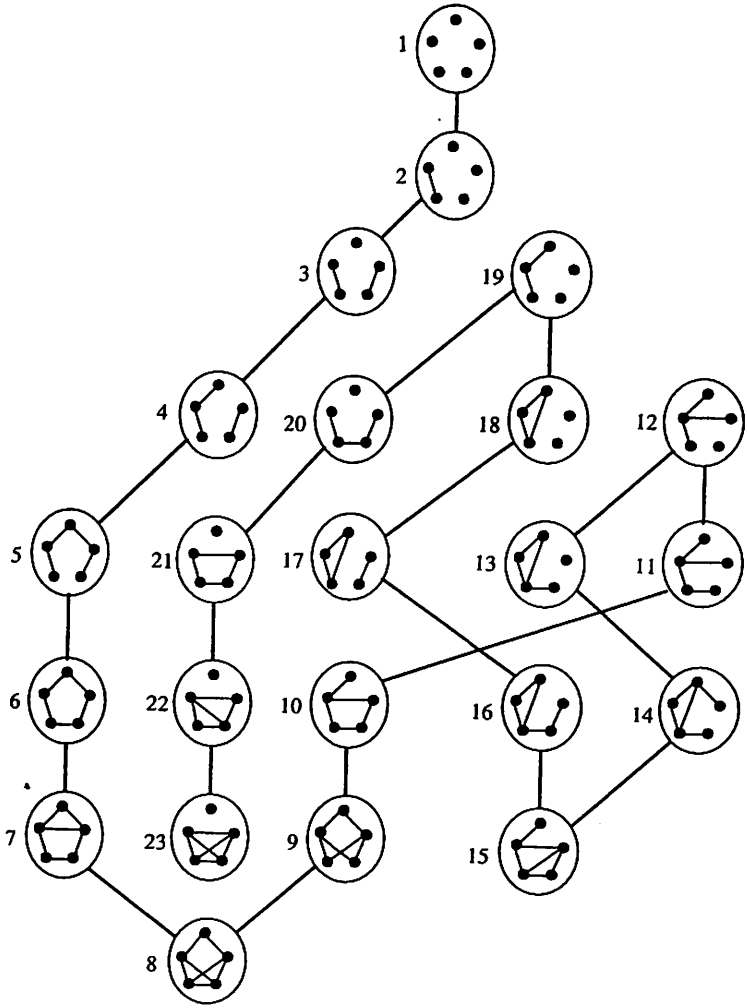
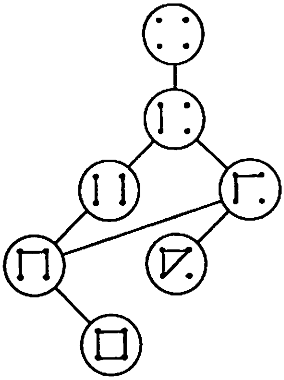
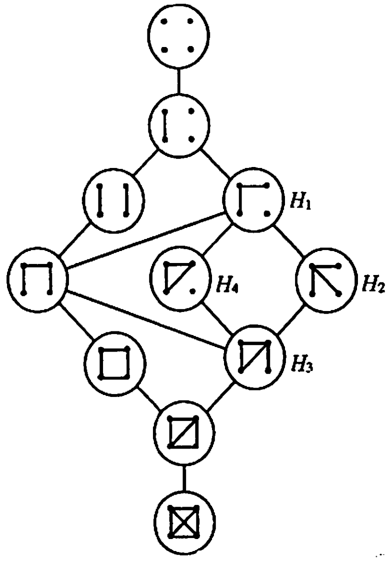


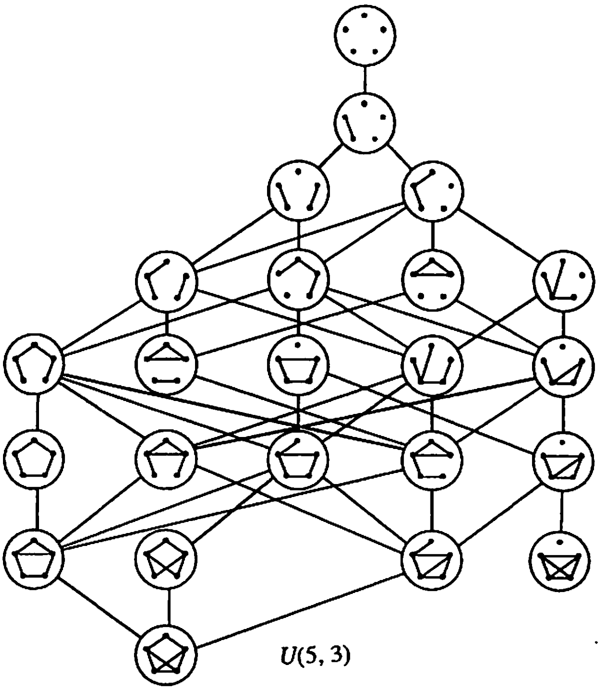
Figure 3. A Hamilton path in $U(5, 3)$



$U(4, 2)$



$U(4, 3)$



$U(5, 3)$

Figure 4. The graphs $U(4, 2)$, $U(4, 3)$, and $U(5, 3)$

Table 1. $N(n, 2)$, $e_2(n)$, $o_2(n)$ and the difference of the latter for $3 \le n \le 20$

n	$N(n, 2)$	$a = e_2(n)$	$b = o_2(n)$	$a - b$
3	4	2	2	0
4	7	4	3	1
5	11	6	5	1
6	19	10	9	1
7	29	15	14	1
8	46	24	22	2
9	70	36	34	2
10	106	54	52	2
11	156	79	77	2
12	232	118	114	4
13	334	169	165	4
14	482	243	239	4
15	686	345	341	4
16	971	489	482	7
17	1357	682	675	7
18	1894	951	943	8
19	2612	1310	1302	8
20	3592	1802	1790	12

Table 2. $N(n, 3)$, $e_3(n)$, $o_3(n)$ and the difference of the latter for $4 \le n \le 17$

n	$N(n, 3)$	$a = e_3(n)$	$b = o_3(n)$	$a - b$
4	11	6	5	1
5	23	12	11	1
6	62	31	31	0
7	150	75	75	0
8	424	214	210	4
9	1165	585	580	5
10	3547	1773	1774	–1
11	10946	5474	5472	2
12	36327	18177	18150	27
13	124380	62191	62189	2
14	449239	224580	224659	–79
15	1680970	840630	840340	290
16	6553568	3277075	3276493	–582
17	26400465	13198356	13202109	–3753

Table 3. The orders of the graphs in the Extended Foster Census

2	4	6	8		440 ABC	446	448 ABC	450
10	14	16	18		456 AB	458	468	474
20 AB	24	26	28		480 ABCD	482	486 ABCD	488
30	32	38	40		494 AB	496	500	504 ABCDE
42	48	50	54		506 AB	512 ABCDEFG	518 AB	536
56 ABC	60	62	64		542	546 AB	554	558
72	74	78	80		566	570 AB	576 ABCD	578
84	86	90	96 AB		582	584	592	600
98 AB	102	104	108		602 AB	608	614	618
110	112 ABC	114	120 AB		620	624 AB	626	632
122	126	128 AB	134		640	648 ABCDEF	650 AB	654
144 AB	146	150	152		660	662	666	672 ABCD EFG
158	162 ABC	168 ABCDEF	182 ABCD		674	680 AB	686 ABC	688
186	192 ABC	194	200		698	702 AB	720 ABCDEF	722 AB
204	206	208	216 ABC		726	728 ABCDEFG	734	744 AB
218	220 ABC	222	224 ABC		746	750	758	762
234 AB	240 ABC	242	248		768 ABCD EFG	774	776	784 AB
250	254	256 ABCD	258		794	798 AB	800	806 AB
266 AB	278	288 AB	294 AB		818	824	832	834
296	302	304	312 AB		840	842	854 AB	864 ABCD
314	326	336 ABCDEF	338 AB		866	872	878	880
342	344	350	360 AB		882 AB	888 AB	896 ABC	906
362	364 ABCDE FG	366	378 AB		912 AB	914	926	936 AB
384	386	392 AB	398		938 AB	942	950	960 ABC
400 AB	402	408 AB	416		962 AB	968	974	976
422	432 ABCDE	434 AB	438		978	992	998	