HSAGA and its application for the construction of near-Moore digraphs ☆

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Abstract

The degree/diameter problem is to determine the largest graphs or digraphs of given maximum degree and given diameter. This paper deals with directed graphs. General upper bounds, called Moore bounds, exist for the largest possible order of such digraphs of maximum degree d and given diameter k. It is known that simulated annealing and genetic algorithm are effective techniques to identify global optimal solutions.

This paper describes our attempt to build a Hybrid Simulated Annealing and Genetic Algorithm (HSAGA) that can be used to construct large digraphs. We present our new results obtained by HSAGA, as well as several related open problems.
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1. Introduction

1.1. Basic concepts

In this paper we consider only finite directed graphs. An interconnection network can be modeled as a *digraph*, where each element can be represented as a vertex and the directed connection between two vertices is described by an *arc*. A digraph has vertex set $V(G)$. The number of vertices is called the *order n* of the digraph, and the number of arcs from a vertex is called the *out-degree d* of the vertex. The *diameter k* is defined to be the length of the largest of the shortest paths between any two vertices. From now on, we denote by $\mathcal{G}(n, d, k)$ the set of all digraphs G of order n, maximum out-degree d, and given diameter k. In this paper we deal with the *degree/diameter problem* [4].

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- *Degree/diameter problem*: Given natural numbers d and k, find the largest possible number of vertices $n_{d,k}$ in a digraph of maximum out-degree d and diameter $\leqslant k$.

Let u be an arbitrary vertex of G and define n_i to be the number of vertices at distance at most i from u. Then we count the maximum number of vertices n_i at distance i from u, $n_i \leqslant d^i$, for $0 \leqslant i \leqslant k$, and consequently,

$$n_{d,k} = \sum_{i=0}^{k} n_i \leqslant 1 + d + d^2 + \cdots + d^k = \begin{cases} \frac{d^{k+1}-1}{d-1} & \text{if } d > 1, \\ k+1 & \text{if } d = 1. \end{cases} \tag{1}$$

The right-hand side of (1), denoted by $M_{d,k}$, is called the *Moore bound* for digraphs, which is the largest possible order (i.e., the number of vertices) of a digraph G of maximum out-degree d and diameter k. If the equality sign holds in (1) then the digraph is called a *Moore digraph*. It is well known that Moore digraphs of degree d, diameter k do not exist for $d \geqslant 2$ and $k \geqslant 2$. This was first proved by Plesník and Znám [8], and in a simpler way by Bridges and Toueg [1] in 1980.

The remainder of this paper is organized as follows. In Section 2, some open problems regarding near-Moore digraphs will be discussed. In Section 3, we will introduce several optimization algorithms, such as Simulated Annealing and Genetic Algorithms, also we would like to propose an optimization algorithms method, called Hybrid Simulated Annealing and Genetic Algorithm (HSAGA). In Section 4, we present some outputting results that we have obtained so far using HSAGA. Finally, further research will be described in Section 5.

2. Open problems

2.1. Relaxed Moore digraphs

It is well known that Moore digraphs exist only for $d = 1$ or $k = 1$. Consequently, we are interested in studying the existence of large digraphs which are in some way 'close' to Moore digraphs. Currently, we are considering relaxing in turn the parameters, namely, the order $M_{d,k}$, the out-degree d, and the diameter k, in order to get close to Moore digraphs.

Definition 2.1. A digraph G is a $(n, \mathcal{S}^+, \mathcal{E}^+)$-*digraph* if G has order n, out-degree sequence $\mathcal{S}^+$ and out-eccentricity sequence $\mathcal{E}^+$.

2.1.1. Relaxing the order
Currently, most research is focusing on finding the best lower and upper bounds of large digraphs, in order to obtain large digraphs, of orders 'close' to the Moore bound with maximum out-degree and given diameter. This kind of large digraph we will call the "order-relaxed Moore digraph".

Definition 2.2. A digraph G is an *order-relaxed Moore digraph*, denoted (n, d, k)-digraph, if G has given diameter k, maximum out-degree d of order $n = M_{d,k} - \delta$, $\delta > 0$.

The problem of obtaining an order-relaxed Moore digraph is as follows.

Problem 2.1. What is the minimum value of δ of an order-relaxed Moore digraph with maximum out-degree d and given diameter k?

2.1.2. Relaxing the out-degree
The problem of relaxing the out-degree to get close to Moore digraphs is still quite open. Here we would like to find digraphs which are 'close' to Moore digraphs, by relaxing the maximum out-degree d. This kind of large digraph will be called an "out-degree-relaxed Moore digraph".

Definition 2.3. A digraph G is an *out-degree-relaxed Moore digraph*, denoted $(M_{d,k}, \mathcal{S}^+, k)$-digraph, if it has $M_{d,k}$ vertices and given diameter k, and $\mathcal{S}^+ = (d^{t_0}, (d+1)^{t_1}, (d+2)^{t_2}, \ldots, (d+m)^{t_m})$.

Currently, we are dealing with a special out-degree sequence $\mathcal{S}^+$ in the $(M_{d,k}, \mathcal{S}^+, k)$-digraph when the digraph G has β vertices of out-degree larger than d, where $t_1 + t_2 + \cdots + t_m = \beta$, minimum out-degree d and maximum out-degree $d + m$, with $0 < m \leqslant M_{d,k} - d - 1$. Furthermore, this special $\mathcal{S}^+$ can be described as $(d^{M_{d,k}-\beta}, (d+1)^{t_1}, (d+2)^{t_2}, \ldots, (d+m)^{t_m})$.

The number of extra arcs is $E = t_1 + 2t_2 + \cdots + mt_m$. We are interested not only in the number of extra arcs E, but in the distribution of these extra arcs.

For the out-degree-relaxed Moore digraphs, we are interested in the following problems.

1. What is the minimum value of E of an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k?
2. What is the minimum value of β in terms of the E, if G is an out-degree-relaxed Moore digraph and $\beta \neq 1$? One extreme case is when $\beta = 1$, that is, when the digraph has one vertex of maximum out-degree $d + E$, and the rest of the vertices all have out-degree d. The corresponding out-degree sequence can be described as $\mathcal{S}^+ = (d^{M_{d,k}-1}, d + E)$ and the problem can be restated as "What is the minimum value of β to what is the minimum value of $d + E$"?
3. What is the minimum value of the maximum out-degree $d + m$, if G is an out-degree-relaxed Moore digraph and $E \neq \beta$? One extreme case is $E = \beta$, that is, the digraph has β vertices of out-degree $d + 1$, and the rest of the vertices all have out-degree d. The corresponding out-degree sequence is $\mathcal{S}^+ = (d^{M_{d,k}-\beta}, (d+1)^{\beta})$. Thus instead of investigating the minimum value of maximum out-degree $d + m$, we can investigate the minimum value of β.

In particular, we are interested in the problems of obtaining out-degree-relaxed Moore digraph for certain special sequences $\mathcal{S}^+$.

Problem 2.2. What is the minimum value of E of an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k?

Problem 2.3. What is the minimum value of β in terms of E, if G is an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k, and $\beta \neq 1$?

Problem 2.4. What is the minimum value of β in terms of E, if G is an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k, and $E = \beta$?

Problem 2.5. What is the minimum value of maximum out-degree $d + m$, if G is an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k, and $E \neq \beta$?

Problem 2.6. What is the minimum value of maximum out-degree $d + E$, if G is an out-degree-relaxed Moore digraph with $M_{d,k}$ vertices and given diameter k, and $\beta = 1$?

2.2. Relaxed digraphs

Currently, there are usually large gaps between the best current lower and upper bounds of order $n_{d,k}$. Let $l_{d,k}$ represent the current best lower bound for the order $n_{d,k}$, and let $u_{d,k}$ represent the current best upper bound for $n_{d,k}$. We are interested in improving the lower bounds to decrease these gaps by obtaining digraphs of order equal to values between $l_{d,k}$ and $u_{d,k}$, given diameter and maximum out-degree. However, currently we are unable to obtain these digraphs and so we begin by obtaining large digraphs, of orders equal to values between $l_{d,k}$ and $u_{d,k}$ and having a given diameter k, and relaxed out-degree d. Obtaining these large digraphs is expected to produce structures which may be useful to utilize in the construction of new digraphs in order to improve the lower bounds for the maximum order of digraphs.

2.2.1. Digraphs of order between $l_{d,k}$ and $u_{d,k}$

We tabulate in Tables 1, 2 and 3, the outstanding potential values of orders larger than those obtained so far, for diameter k up to 10, and for maximum degree $d = 2, 3$ and 4. The 'Largest known order' column gives the order of

Table 1
Possible values of $n_{2,k}$ for $2 \leqslant k \leqslant 10$

k	Largest known order	Possible larger values of order
2	6	–
3	12	–
4	25	26–28
5	50	51–60
6	100	101–124
7	200	201–252
8	400	401–508
9	800	801–1020
10	1600	1601–2044

Table 2
Possible values of $n_{3,k}$ for $2 \leqslant k \leqslant 10$

k	Largest known order	Possible larger values of order
2	12	–
3	36	37–38
4	108	109–119
5	324	325–362
6	972	973–1091
7	2961	2962–3278
8	8748	8749–9839
9	26,244	26,245–29,522
10	78,732	78,733–88,571

Table 3
Possible values of $n_{4,k}$ for $2 \leqslant k \leqslant 10$

k	Largest known order	Possible larger values of order
2	20	–
3	80	81–84
4	320	321–340
5	1280	1281–1364
6	5120	5121–5460
7	20,480	20,481–21,844
8	81,920	81,921–87,380
9	327,680	327,681–349,524
10	1,310,720	1310,721–1,398,100

the current largest known digraph of the given maximum out-degree d and diameter k. The possible larger orders, between the current known lower bounds and current best upper bounds, are tabulated under the heading 'Possible larger values of order'. Furthermore, similar tables could also be made for degrees $d > 4$.

2.2.2. Relaxing the out-degree

We begin this subsection by defining a $(n, \mathcal{S}^+, k)$-digraph, where $l_{d,k} < n \leqslant u_{d,k}$, to represent a digraph of order n, with given diameter k, and a relaxed maximum out-degree d.

Definition 2.4. A digraph G is a *out-degree-relaxed digraph*, denoted by $(n, \mathcal{S}^+, k)$-digraph, if G has n vertices, $l_{d,k} < n \leqslant u_{d,k}$, given diameter k, and $\mathcal{S}^+ = (d^{t_0}, (d+1)^{t_1}, (d+2)^{t_2}, \ldots, (d+m)^{t_m})$.

Currently, we are dealing with special out-degree sequences $\mathcal{S}^+$ in the $(n, \mathcal{S}^+, k)$-digraph. Let G have β vertices of out-degree larger than d, $(t_1 + t_2 + \cdots + t_m = \beta)$, minimum out-degree d and maximum out-degree $d + m$, $0 <$

$m \leqslant n - d - 1$. The out-degree sequence $\mathcal{S}^+$ can then be described as $(d^{n-\beta}, (d+1)^{t_1}, (d+2)^{t_2}, \ldots, (d+m)^{t_m})$. The number of extra arcs in a $(n, \mathcal{S}^+, k)$-digraph is $E = t_1 + 2t_2 + \cdots + mt_m$.

Problem 2.7. What is the minimum value of E, if G is a $(n, \mathcal{S}^+, k)$-digraph with n vertices, $l_{d,k} < n \leqslant u_{d,k}$, and given diameter k?

3. Optimization algorithms

3.1. Simulated annealing

The algorithm is based upon that of Metropolis et al. [5], which was originally proposed as a means of finding the equilibrium configuration of a collection of atoms at a given temperature. See also Cerny [2]. The connection between this algorithm and mathematical minimization was first noted by Pincus [7]. However, it was Kirkpatrick et al. [3] who proposed that it form the basis of an optimization technique for combinatorial (and other) problems.

Simulated Annealing (SA) is a means of finding good solutions to combinatorial optimization problems. The basic operation in this technique is a *move*. A move is a transition from one element of the solution space to another element. In this report, a move means inserting an arc between two randomly generated nonadjacent vertices x and y and removing one of the arcs from x, depending on their *cost*. The *cost* of a vertex x, denoted by $c(x)$, is the number of unique vertices reached by x at most in k steps. Assume m and n are out-neighbors of the vertex x and $c(m)$ is less than $c(n)$. If $c(y)$ more than $c(m)$, we must remove the arc between x and m, and insert an arc from x to y. Otherwise, we accept the arc $(x \rightarrow y)$ with probability $= e^{-\triangle E/T}$, where T is a global time-varying parameter called the *temperature* and $\triangle E$ is the increase in *cost* (i.e., $c(y) - c(m)$) that would result form this prospective move.

The pseudo code [9] for our implementation is given below. In the inner loop, move is selected at random. A limited number of move are accepted at each *temperature* level. For better results in terms of small diameters, we would use larger numbers of move. In our study, we use $20|V(G)|$ as the maximum number of moves. Furthermore, there is a limit on the number of attempted moves at each temperature. For each accepted move, we want to attempt no more than 60 moves. Once the maximum number of accepted moves or the maximum number of attempted moves has been reached, the temperature is lowered and a new iteration begins.

```
Simulated Annealing(G)
   temp = initial_temp = 1.0
   Cool_rate = 0.95
   Max_moves = 20 * |V|                    // maximum number of moves
   Max_attempted_moves = 60 * max_moves  // maximum number of attempted moves
   Max_frozen = 100
   frozen = 0
   randomly create a digraph based on given order and out-degree
   While (frozen <= Max_frozen)
       moves = 0                // number of moves
       attempted_moves = 0    // number of attempted moves
       While ((moves <= Max_moves) and (attempted_moves <= Max_attempted_moves))
           increase attempted_moves
           randomly select two non-adjacent vertices
           If the random vertices are accepted
              do move() and increase moves
              // new digraph's diameter is equal to required diameter k
              If (k(G new) == k required)
                 return the improved solution, and end Simulated Anneal(G)
              End if
           End if
       End while
       temp = temp * Cool_rate
       If(attempted_moves > Max_attempted_moves)
```

```
            increase frozen
        End if
   End while
End Simulated Annealing(G)
```

3.2. Genetic Algorithm

Genetic Algorithm (GA) is a search technique for global optimization in a complex search space. As the name suggests, GA employs the concepts of natural selection and genetics [6].

In GA, search space is composed of all the possible solutions to the problem. A solution in the search space is represented by a sequence of 0's and 1's. This solution is referred to as the *chromosome* in the search space. Each chromosome has an associated objective function value called *fitness value*. A good chromosome is one that has high/low fitness value depending on the problem (maximization/minimization). A set of chromosomes and the associated fitness values is called the *population*.

There are five basic functions inside of GA. *Fitness* is used to evaluate the fitness value of each chromosome in the current population. *Selection* is used to choose two parent chromosomes from the current population according to their fitness values. *Crossover* is used to cross over the two parents to form two new offspring based on *Crossover_rate*, which is the odds of a parent being selected for the crossover operation. Actually, if no crossover is performed, then offsprings are created as the exact copies of parents. Furthermore, the *Mutation* is used to mutate new offspring at each position in chromosome in terms of *Mutation_rate*, which specifies the odds that a given position in a offspring will be mutated. Finally, *Test* is used to evaluate whether or not the new offspring satisfies the end condition.

The pseudo code of the general GA procedure is given below.

```
Genetic Algorithm(G)
  Crossover_rate = 0.95, Mutation_rate = 0.03
  Curr_population_size = 200
  Create an empty new population
  Found_solution = false
  do Initial_Population() // Randomly generate a current population with
                             200 chromosomes.
  While (Found_solution = false)
    do Fitness()
    While (Curr_population_size < 0)
      do Selection()
      do Crossover()
      do Mutation()
      If (Test() = true)
         Return the improved solution
         Found_solution = true // End Genetic Algorithm(G)
      Else (Test() = false)
         do Accepting() // Place new offsprings in the new population.
         Curr_population_size = Curr_population_size - 2
      End if
    End while
    do Replace() // Use new generated population to replace the
                    current population for a further run of the GA.
    Curr_population_size = 200
  End while
End Genetic Algorithm(G)
```

3.3. Hybrid simulated annealing and genetic algorithm

We introduce an optimization algorithm method: the *Hybrid simulated annealing and genetic algorithms* (HSAGA). The general idea of HSAGA in our study is that an initial digraph is created at the beginning, and used
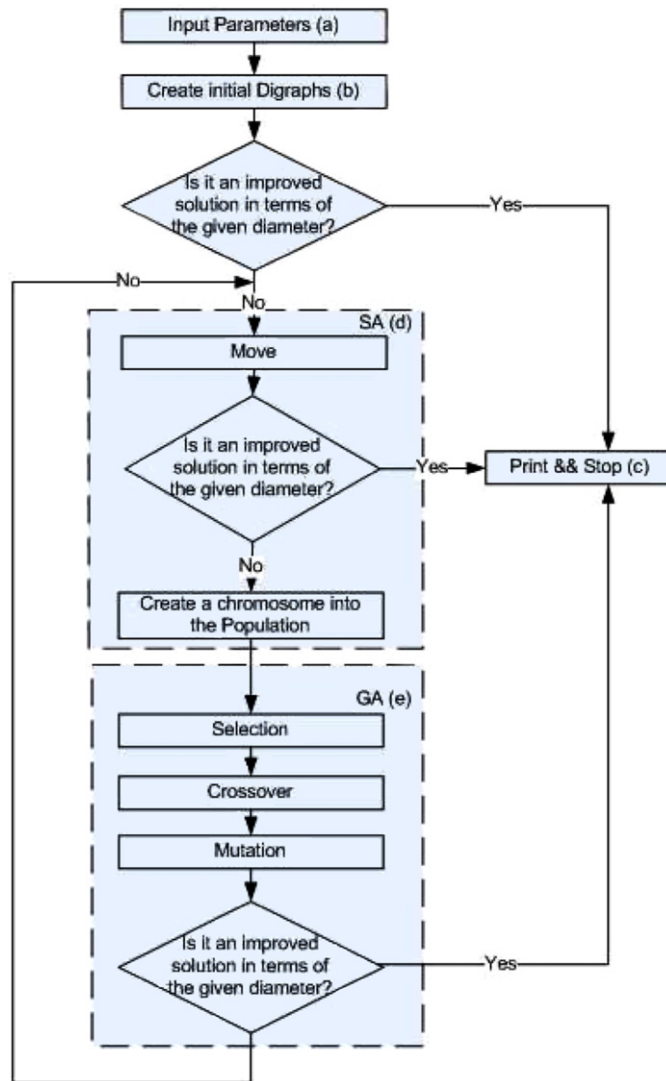
Fig. 1. Basic structure of HSAGA.

as the initial digraph input into SA. SA will terminate if the generated solution is satisfied in terms of given diameter after move, otherwise, the population of candidate solutions will be obtained. Furthermore, the set of elite individuals of the population is chosen by a selection procedure of GA according to their evaluation fitness values, following genetic operations consisting of crossover and mutation. The basic processes of HSAGA are shown in Fig. 1, and the details of each process are described below.

(a) Input parameters into our program, such as the out-degree, required minimum diameter, as well as *cooling rate*, which controls the decreasing of temperature, and *population's size*, that is, the numbers of chromosome, and so on.
(b) Create an initial base digraph in terms of given out-degree and diameter by using the construction technique, known as the generalized Kautz digraphs. Every digraph is represented by an adjacency matrix.
(c) If the current digraph is an improved digraph in terms of given diameter, then we terminate our process and output the result.
(d) Otherwise, put the current digraph into the method called SA. During its processing, SA will execute move to optimize the current digraph, We have a valuation function to test whether or not the diameter of the generated

Table 4
The number of central vertices and the minimum values of diameter k obtained from our
tests when $d = 2$ and $n \leqslant 18$

n	SA		GA		HSAGA	
	c	k	c	k	c	k
1	0	0	0	0	0	0
2	2	1	2	1	2	1
3	3	1	3	1	3	1
4	4	2	4	2	4	2
5	4	3	5	2	5	2
6	6	2	6	2	6	2
7	7	3	7	3	7	3
8	8	3	8	3	8	3
9	9	3	9	3	9	3
10	9	4	9	4	**10**	**3**
11	7	4	6	4	**11**	**3**
12	5	4	5	4	**12**	**3**
13	12	5	13	4	**13**	**4**
14	14	4	14	4	**14**	**4**
15	13	5	14	5	**15**	**4**
16	11	5	14	5	**16**	**4**
17	10	5	9	5	**17**	**4**
18	8	5	10	5	**18**	**4**

digraph matches the desired given diameter. If yes, then the process will stop and go to Step c. Otherwise, it will create a chromosome, based on its fitness value, which is represented by the number of reached central vertices by the current generated digraph, then store each chromosome into the population. If we fix the population size as 200, HSAGA will obtain a population of the first 200 best chromosomes, based on their fitness values.

(e) Input the current population into GA functions consisting of selection, crossover and mutation, in order to obtain an improved solution, that is, a digraph whose diameter is equal to the given diameter. It is well known that GA never guarantees to generate a best solution, no matter what is the running time. So if GA could not give us an improved digraph at the end of the running time, we will select a current best chromosome, and input it back to SA, until the improved solution is found with respect to the given diameter.

4. Results

In order to make comparisons with other important optimization algorithms, including SA, GA, and HSAGA, which could be used to solve the degree/diameter problems, we have performed various experiments. The best experimental results that we have obtained are given in Table 4. A central vertex, denoted by c, is a vertex of eccentricity equal to the radius of the digraph. It is easy to observe that neither of the SA and GA has been effective for this problem. In other words, SA and GA have not given us the minimum diameter and maximum number of central vertices for orders greater than 10. However, combining SA and GA in the hybrid method has given more encouraging results.

5. Out-degree-relaxed Moore digraph

Using HSAGA, we have obtained out-degree-relaxed Moore digraphs of diameter $2 \leqslant k \leqslant 6$ and most, but not all, vertices with out-degree $d = 2$ and with order equal to the Moore bounds $M_{2,k}$. For example, there are a few out-degree-relaxed Moore digraphs are listed below (see Figs. 2–4). Surprisingly, we found five nonisomorphic out-degree-relaxed Moore digraphs with the same out-degree sequences, diameter $k = 3$ and order 15, but with different in-degree sequences (see Fig. 4).

In order to summarize our results concerning our out-degree-relaxed Moore digraphs and current results on order-relaxed Moore digraphs, we have created Table 5. In this table, we list current largest digraphs of order n with its current best δ by relaxing the order, and out-degree sequence $\mathcal{S}^+$ with its current minimum number of extra arcs E and current minimum β, obtained by relaxing the out-degree $d = 2$ and given diameter $2 \leqslant k \leqslant 6$.
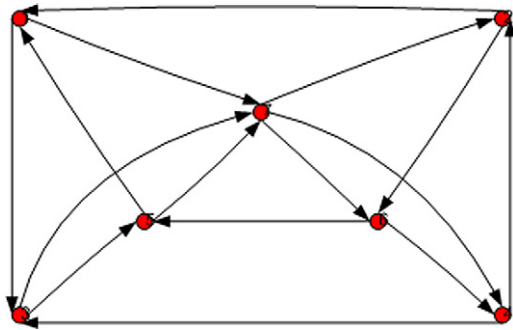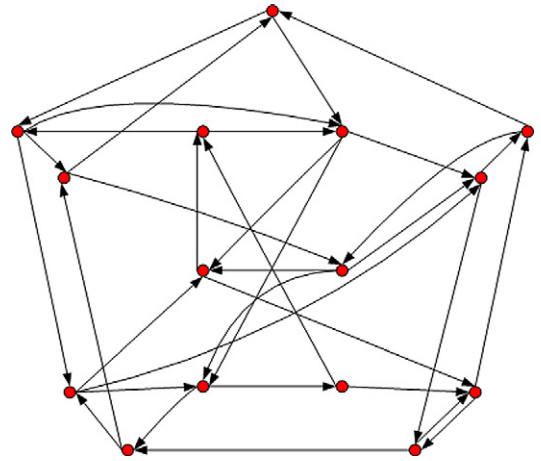
Fig. 2. $G \in G(7, (2^6, 3), 2)$.

Fig. 3. $G \in G(15, (2^{12}, 3^3), 3)$.

Table 5
The current largest digraphs of order n with current best δ by relaxing the order, and the current minimum number of extra arcs E, current minimum β, with out-degree sequences $\mathcal{S}^+$, for $d = 2$ and given $2 \leqslant k \leqslant 6$

	Order-relaxed			Out-degree-relaxed			
k	n	d	δ	$M_{d,k}$	$\mathcal{S}^+$	E	β
2	6	2	1	7	$(2^6, 3)$	1	1
3	12	2	3	15	$(2^{12}, 3^3)$	3	3
					$(2^{14}, 5)$	3	1
4	25	2	6	31	$(2^{27}, 3^4)$	4	4
					$(2^{14}, 10)$	8	1
5	50	2	13	63	$(2^{57}, 3^6)$	6	6
6	100	2	27	127	$(2^{118}, 3^9)$	9	9

Table 6
The current minimum number of extra arcs E, current minimum β, and its corresponding $\mathcal{S}^+$, with respect to the out-degree, where $d = 2$, $k = 4$ and n, such that $l_{2,4} < n \leqslant u_{2,4}$

Out-degree-relaxed				
k	n	$\mathcal{S}^+$	E	β
4	26	$(2^{24}, 3^2)$	2	2
		$(2^{25}, 5)$	3	1
4	27	$(2^{24}, 3^3)$	3	3
		$(2^{26}, 6)$	4	1
4	28	$(2^{25}, 3^3)$	3	3
		$(2^{27}, 8)$	6	1

6. Out-degree-relaxed digraphs

Using HSAGA, we have also obtained some large digraphs with order n, for example, $n = 26, 27$ and 28, that is, $l_{2,4} < n \leqslant u_{2,4}$, and given diameter $k = 4$, by relaxing out-degree $d = 2$ (see Figs. 5–10).

To summarize, we list the current minimum extra arcs E, current minimum β, and the corresponding out-degree sequence $\mathcal{S}^+$ in Table 6.

(a) G_1 ⬜ (b) G_2
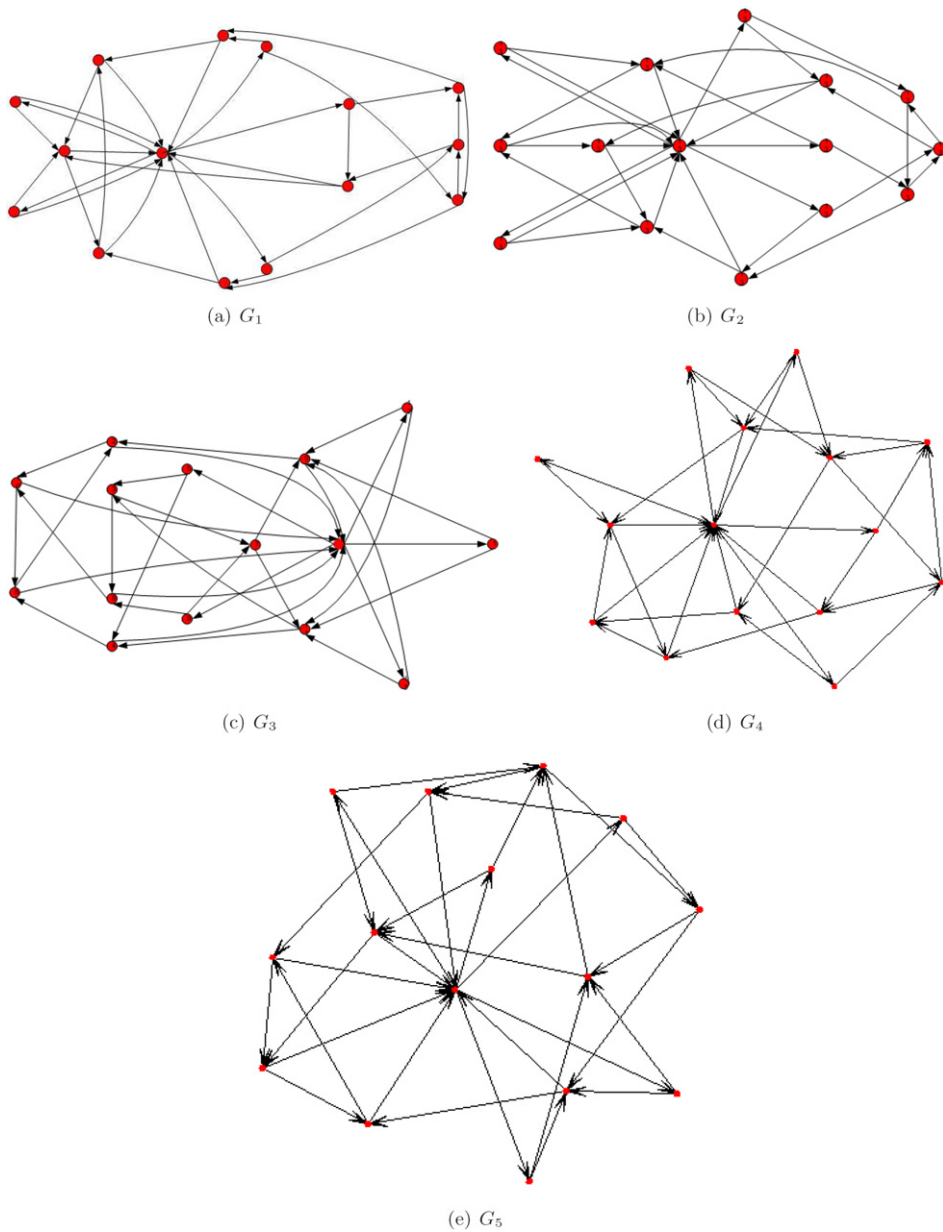
(c) G_3 ⬜ (d) G_4

(e) G_5

Fig. 4. Five nonisomorphism digraphs $\in G(15, (2^{14}, 5), 3)$.

7. Further research

In preliminary results, we have obtained some out-degree-relaxed Moore digraphs and some out-degree-relaxed digraphs of orders between $l_{2,4}$ and $u_{2,4}$, by using HSAGA. In order to improve its efficiency, we shall next modify our HSAGA to *Parallel Hybrid Simulated Annealing and Genetic Algorithm*, denoted by PHSAGA, so that the issue of time consumed for the running of HSAGA can be solved.

In addition, it may be possible to implement PHSAGA to deal with undirected graphs as well, that is, finding degree-relaxed Moore graphs, in order to get close to Moore graphs. We also consider to search for large graphs of orders between the best current lower and upper bounds for the order $n_{\Delta, D}$, with maximum degree Δ and given diameter D, by using PHSAGA combined with other construction techniques, to improve the current lower bounds of undirected graphs.
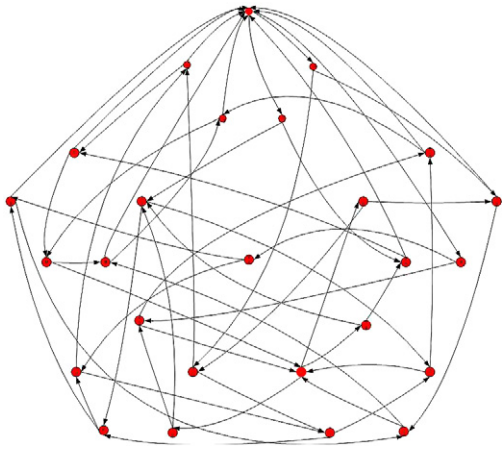
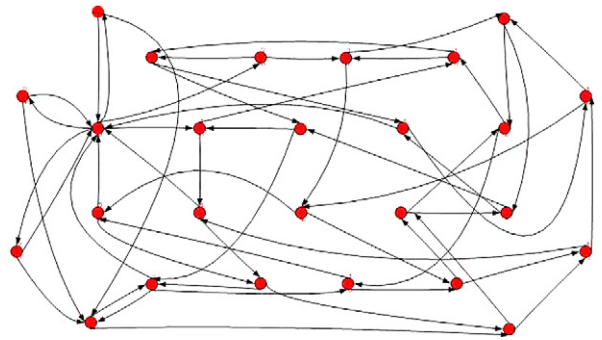Fig. 5. $G \in G(26, (2^{24}, 3^2), 4)$.
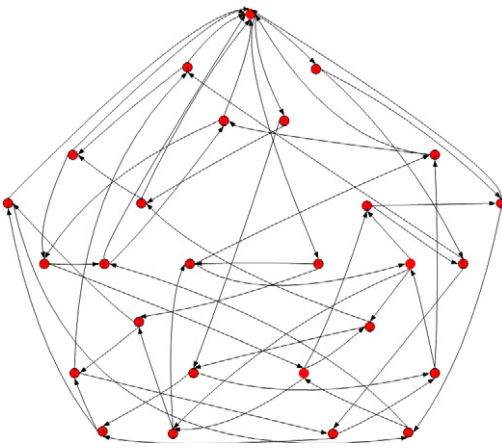

Fig. 6. $G \in G(26, (2^{25}, 5), 4)$.

Fig. 7. $G \in G(27, (2^{24}, 3^3), 4)$.

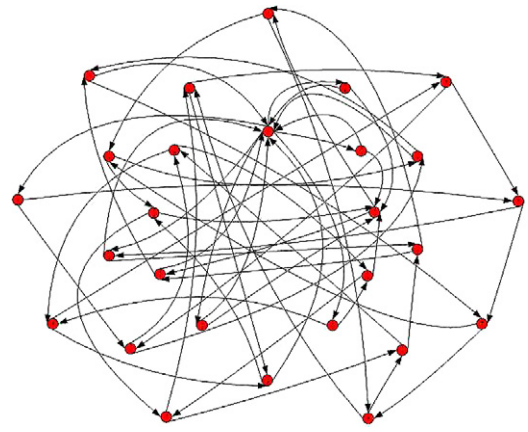

Fig. 8. $G \in G(27, (2^{26}, 6), 4)$.

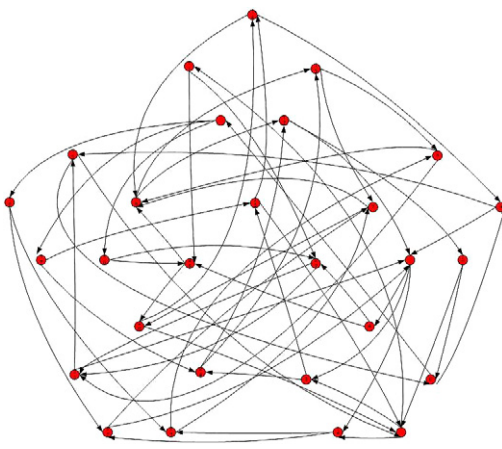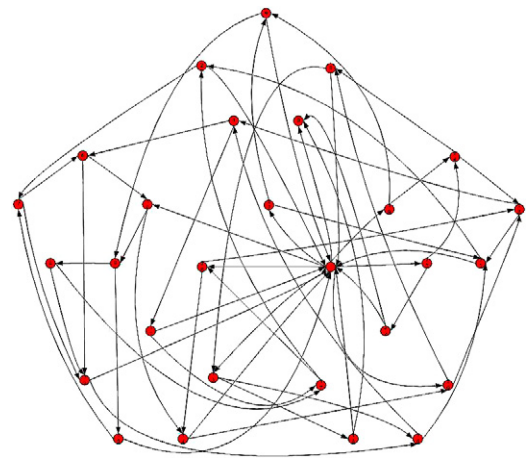Fig. 9. $G \in G(28, (2^{25}, 3^3), 4)$.

Fig. 10. $G \in G(28, (2^{27}, 8), 4)$.

Acknowledgements

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