Fast Generation of Regular Graphs and Construction of Cages

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Abstract: The construction of complete lists of regular graphs up to isomorphism is one of the oldest problems in constructive combinatorics. In this article an efficient algorithm to generate regular graphs with a given number of vertices and vertex degree is introduced. The method is based on orderly generation refined by criteria to avoid isomorphism checking and combined with a fast test for canonicity. The implementation allows computing even large classes of graphs, like construction of the 4-regular graphs on 18 vertices and, for the first time, the 5-regular graphs on 16 vertices. Also in cases with given girth, some remarkable results are obtained. For instance, the 5-regular graphs with girth 5 and minimal number of vertices were generated in less than 1 h. There exist exactly four (5, 5)-cages. © 1999 John Wiley & Sons, Inc. J Graph Theory 30: 137–146, 1999

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1. INTRODUCTION

Let $\mathcal{G}_n$ denote the set of simple labeled graphs with vertex set $\{1,\ldots,n\}$. The subset of k-regular graphs, i.e., those graphs where each vertex has degree exactly

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k, is called $\mathcal{R}_{n,k}$. $\Gamma \in \mathcal{G}_n$ is described by the set of its edges:

$$\Gamma = \{e_1, \ldots, e_t\} \subseteq \binom{\{1, \ldots, n\}}{2} =: X_n.$$

If $e = (v, w) \in X_n$ denotes an edge, always $v < w$ is assumed. The symmetric group S_n acts on X_n and, therefore, induces actions on $\mathcal{G}_n$ and $\mathcal{R}_{n,k}$. $S_n \backslash\backslash \mathcal{G}_n$ and $S_n \backslash\backslash \mathcal{R}_{n,k}$ denote the orbits of these actions. By definition, two labeled graphs are isomorphic if and only if they belong to the same orbit. Our aim is to compute a set of orbit representatives of $S_n \backslash\backslash \mathcal{R}_{n,k}$ (cf. [10]).

2. ORDERLY GENERATION

To find a set of orbit representatives, Read's technique of orderly generation [13] is used. X_n is ordered in the following way: For $e = (v, w), e' = (v', w') \in X_n$, we define

$$e < e' :\Leftrightarrow v < v' \vee (v = v' \wedge w < w').$$

This induces a lexicographic order on $\mathcal{G}_n$: Let $\Gamma, \Gamma' \in \mathcal{G}_n$ with $\Gamma = \{e_1, \ldots, e_t\}, \Gamma' = \{e'_1, \ldots, e'_{t'}\}$, and $e_1 < \cdots < e_t, e'_1 < \cdots < e'_{t'}$. Then

$$\Gamma < \Gamma' :\Leftrightarrow (\exists i \leq \min\{t, t'\} : e_j = e'_j \forall j < i \wedge e_i < e'_i) \vee (t < t' \wedge e_j = e'_j \forall j \leq t).$$

The canonical orbit representatives are defined to be minimal in their orbit:

$$\mathrm{rep}_<(S_n \backslash\backslash \mathcal{G}_n) := \{\Gamma \in \mathcal{G}_n | \forall \pi \in S_n : \Gamma \leq \Gamma^\pi\},$$

$$\mathrm{rep}_<(S_n \backslash\backslash \mathcal{R}_{n,k}) := \{\Gamma \in \mathcal{R}_{n,k} | \forall \pi \in S_n : \Gamma \leq \Gamma^\pi\}.$$

The following theorem [9] provides the key for the computation of the minimal orbit representatives.

Theorem 2.1. *If* $\Gamma \in$ *rep*$_<(S_n \backslash\backslash \mathcal{G}_n)$, *each* $\Gamma_1 \subset \Gamma$ *with* $\Gamma_1 < \Gamma$ *fulfills* $\Gamma_1 \in$ *rep*$_<(S_n \backslash\backslash \mathcal{G}_n)$.

Proof. Let $\Gamma = \Gamma_1 \cup \Gamma_2$ and $\Gamma_1 \notin \mathrm{rep}_<(S_n \backslash\backslash \mathcal{G}_n)$ and $\Gamma_1 < \Gamma$. Then $\Gamma_1^\pi < \Gamma_1$ for some $\pi \in S_n$. Let $\Gamma_1^\pi = \{e_1, \ldots, e_t\}, e_1 < \cdots < e_t$ and $\Gamma_1 = \{e'_1, \ldots, e'_t\}, e'_1 < \cdots < e'_t$. By $\Gamma_1^\pi < \Gamma_1$ exists $i := \min\{j | e_j < e'_j\}$. Now $\Gamma^\pi = \Gamma_1^\pi \cup \Gamma_2^\pi \supseteq \{e_1, \ldots, e_i\}$, and $\Gamma^\pi < \Gamma_1 < \Gamma$. This is a contradiction to the minimality of Γ. ∎

Algorithm 2.1. Based on Theorem 2.1, we can formulate a simple backtracking algorithm to compute $\mathrm{rep}_<(S_n \backslash\backslash \mathcal{R}_{n,k})$ starting with Ordrek ({(1, 2)}). Ordrek is defined as follows.

Ordrek (Γ)

1. Check whether Γ can be extended to a k-regular Graph on n vertices; if not: return.

2. Check, if $\Gamma \in \text{rep}_<(S_n\backslash\backslash\mathcal{G}_n)$; if not: return.
3. If $\Gamma \in \mathcal{R}_{n,k}$: add Γ to the output; return.
4. For each $e \in X_n$ with $e > \max\{e' \in \Gamma\}$, call Ordrek $(\Gamma \cup \{e\})$ with increasing e.

An element of $\mathcal{R}_{n,k}$ is constructed only if Γ contains exactly $\frac{nk}{2}$ edges. At the intermediate stages we just have $\Gamma \in \mathcal{G}_n$. Of course, any vertex should have degree at most k. Further necessary conditions for step 1 can be obtained by taking row and column sums of the adjacency matrix into account (cf. [12]). Indeed there seems to be no necessary and sufficient criterion that is easy to check to decide at any stage whether Γ can become an element of $\mathcal{R}_{n,k}$ by inserting further edges.

The most time-consuming part is step 2: the minimality testing procedure. From the naive point of view, one has to look at any permutation of S_n. Although algebraic and combinatorial methods are used to increase the efficiency, such tests remain quite expensive. For this reason they should be avoided as often as possible. The algorithm checks minimality after each insertion of a new edge. This means that graphs that are added to the output last have to pass the minimality test several times. On the other hand, minimality tests for graphs that cannot be extended to regular graphs should be omitted. It turns out to be more efficient to check minimality only when an element of $\mathcal{R}_{n,k}$ is computed. Unfortunately, then the set of candidates for the minimality test grows much faster than the number of minimal orbit representatives. Further efforts must aim to reduce this set of candidates.

Definition 2.1. For $\Gamma \in \mathcal{G}_n$ and $1 \le i < n$, let $\Gamma_i := \{e = (v, w) \in \Gamma | v = i\}$,

$$C_1 := \{\pi \in S_n | \pi(1) = 1\},$$

$$N_i := \{\pi \in C_i | \Gamma_i^\pi = \Gamma_i\}, \text{ and}$$

$$C_{i+1} := \{\pi \in N_i | \pi(i+1) = i+1\}.$$

By Definition, $\Gamma = \cup_{i=1}^{n-1}\Gamma_i, \Gamma_i \cap \Gamma_j = \emptyset \ (i \ne j)$ and with $1 \le i < j < n$: $e \in \Gamma_i, e' \in \Gamma_j \Rightarrow e < e'$. The following lemma shows a necessary criterion for $\Gamma \in \mathcal{G}_n$ being minimal. It is applied after every insertion of a new edge at step 4.

Lemma 2.1 (R. Grund)**.** For $\Gamma \in \text{rep}_<(S_n\backslash\backslash\mathcal{G}_n)$, we have

$$\forall i < n : \forall \pi \in C_i \colon \Gamma_i \le \Gamma_i^\pi. \quad (*)$$

Proof. Let i_0 be the smallest i that does not fulfill (*), i.e., $\exists \tau \in C_{i_0}$: $\Gamma_{i_0}^\tau < \Gamma_{i_0}$. Because of $C_{i_0} \le N_j \ \forall j < i_0$, we have $\Gamma_j^\tau = \Gamma_j \ \forall j < i_0$. Therefore, $\Gamma^\tau < \Gamma$, a contradiction to the minimality of Γ. ∎

Graphs with the property (*) are called semi-canonic in the sense of [6]. Because each group C_i and N_i is a Young subgroup of S_n, these groups are easy to compute and semi-canonicity can be achieved during insertion of the edges (cf. [5]). A further reduction of the candidate set based on a specific property of the chosen canonical form is obtained by the following.

Lemma 2.2 (G. Brinkmann). If $\Gamma \in \text{rep}_<(S_n \backslash\backslash \mathcal{R}_{n,k})$, then there exists a cycle of minimal length in Γ containing vertices 1, 2, and 3.

A proof can be found in [1], where also the construction of such a cycle and the application of the lemma are described. For instance, Fig. 1 shows two semi-canonical graphs on 6 vertices. By Lemma 2.2, nonminimality is detected and the minimality tests can be avoided. This criterion is most effective in the case of cubic graphs and becomes less important for higher degree (e.g., reduction of candidate set for $n = 18, k = 3$ by factor 10, for $n = 14, k = 4$ by factor 4). The main reason for this behavior is the ratio of small cycles that is increased with the maximum possible degree.

Because the girth is an important invariant of a regular graph and many graph-theoretical questions about regular graphs require a certain minimal girth, it can be important to be able to construct only k-regular graphs with a fixed lower bound g of the girth. To be able to apply Lemma 2.2, we have to know the girth of the graph under consideration at any stage of the computation. Obviously by inserting further edges the girth cannot be increased. Once a graph with girth less than g is obtained, one can backtrack. This simple consideration shows a very straightforward way to construct only k-regular graphs with girth at least g.

3. TEST FOR MINIMALITY

This test has to decide whether a given $\Gamma \in \mathcal{R}_{n,k}$ fulfills

$$\Gamma \leq \Gamma^\pi \quad \forall \pi \in S_n.$$

The centralizer of $1, \ldots, i$ is

$$U_i := \{\pi \in S_n | \pi(1) = 1, \ldots, \pi(i) = i\}.$$

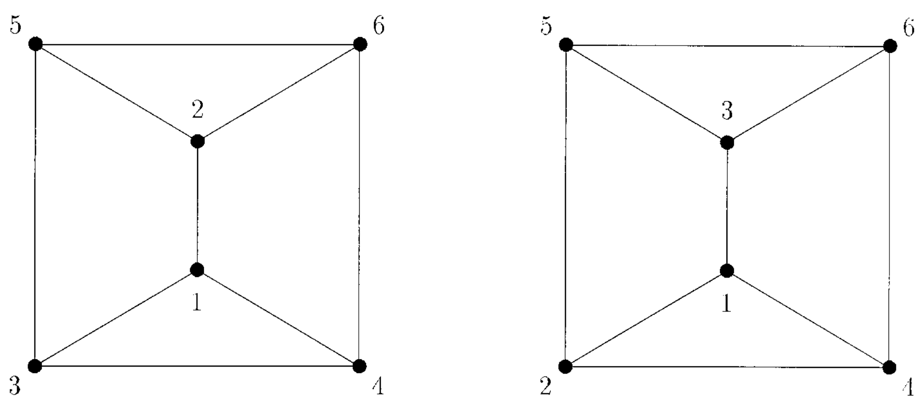

FIGURE 1. Semi-canonical graphs where Lemma 2.2 can be applied.

We have the following chain of subgroups (Sims chain, [14], [11]):

$$S_n =: U_0 \geq U_1 \geq U_2 \geq \cdots \geq U_{n-1} = (\mathrm{id}).$$

Now we consider each of these subgroups as a disjoint union of left cosets:

$$U_{i-1} = \bigcup_{j=i}^{n} (i,j)U_i, \qquad i = 1, \ldots, n-1.$$

The transpositions (i,j) are representatives of left cosets; (i,i) denotes the identity. Any $\pi \in S_n$ can be written in exactly one way as a product of such transpositions:

$$\pi = \prod_{i=1}^{n-1} (i, j_i), \qquad i \leq j_i \leq n, 1 \leq i < n.$$

Algorithm 3.1. Now you can run through S_n as follows: Start at the smallest centralizer U_{n-1}, then run through the difference $U_{n-2} - U_{n-1}$. When all elements of U_{n-2} are visited, you can go on with $U_{n-3} - U_{n-2} \cdots$

Naivetest (Γ)**.** Run through S_n in the way described above. Decide whether

$$\Gamma \leq \Gamma^{(1,j_1)(2,j_2)\cdots(n-1,j_{n-1})}, \qquad i \leq j_i \leq n, 1 \leq i < n,$$

if not: return (not minimal).
We still have to consider any permutation of S_n. A first improvement is achieved by the following.

Lemma 3.1 (R. Grund)**.** For $j > i$, let $\pi \in U_i$ be the first permutation found when running through $(i,j)U_i$ with $\Gamma^{(i,j)\pi} = \Gamma$. Then $\Gamma \leq \Gamma^{(i,j)\sigma}\ \forall \sigma \in U_i$.

Proof. We have $\Gamma^\tau \geq \Gamma\ \forall \tau \in U_i$ (by definition of naivetest). Then for $\sigma \in U_i$ we obtain $\Gamma^{(i,j)\sigma} = \Gamma^{\pi^{-1}\sigma} \geq \Gamma$. ∎

The remaining elements of $(i,j)U_i$ may be neglected and testing is continued at the next coset. This way we get a Sims chain of the automorphism group of the graph, provided that it is a minimal orbit representative. This is an important feature, if we use the graphs as input for further construction algorithms like the one introduced in [7] and [8]. For further refinements to the minimal testing procedure, see [6] and [12].

Even if the candidate is not minimal, you gain valuable information: a necessary condition for the canonicity of the lexicographic successors.

Lemma 3.2 (R. Grund)**.** Let $\Gamma \in \mathcal{G}_n$ be not minimal, $\Gamma = \{e_1, \ldots, e_t\}$ with $e_1 < e_2 < \cdots < e_t$. Then there exists $\pi \in S_n$ and $i < t$ with $\Gamma > \Gamma^\pi = \{e_1, \ldots, e_i,\ e'_{i+1}, \ldots, e'_t\}$ and $e_{i+1} > e'_{i+1}$. Let $\{e_1^{\pi^{-1}}, \ldots, e_i^{\pi^{-1}},\ e'^{\pi^{-1}}_{i+1}\} = \{e_{j_1}, \ldots, e_{j_{i+1}}\}$ with $1 \leq j_l \leq t$ for $l = 1, \ldots, i+1$. Let $r := \max\{j_1, \ldots, j_{i+1}, i+1\}$, then each $\tilde{\Gamma} \in \mathcal{G}_n$ with $\tilde{\Gamma} = \{e_1, \ldots, e_r, \tilde{e}_{r+1}, \ldots, \tilde{e}_s\}, e_1 < \cdots < e_r < \tilde{e}_{r+1} < \cdots < \tilde{e}_s$ is also not minimal.

TABLE I. Connected regular graphs.

n	k	Graphs	Candidates	Cand./Graph	CPU-time
4	3	1	1	1.00	0.0 s
6	3	2	2	1.00	0.0 s
8	3	5	10	2.00	0.0 s
10	3	19	37	1.95	0.0 s
12	3	85	214	2.52	0.0 s
14	3	509	1406	2.76	0.1 s
16	3	4060	10432	2.57	1.0 s
18	3	41301	96279	2.33	10.8 s
20	3	510489	1079585	2.11	2 min 19 s
22	3	7319447	14341762	1.96	34 min 44 s
24	3	117940535	217873241	1.85	9 h 43 min
5	4	1	1	1.00	0.0 s
6	4	1	1	1.00	0.0 s
7	4	2	5	2.50	0.0 s
8	4	6	14	2.33	0.0 s
9	4	16	57	3.56	0.0 s
10	4	59	219	3.71	0.0 s
11	4	265	997	3.76	0.1 s
12	4	1544	5194	3.36	0.3 s
13	4	10778	33139	3.07	2.5 s
14	4	88168	251546	2.85	22.8 s
15	4	805491	2177590	2.70	3 min 35 s
16	4	8037418	20656320	2.57	35 min 59 s
17	4	86221634	212449363	2.46	6 h 28 min
18	4	985870522	2354685107	2.39	3 d 2 h
6	5	1	1	1.00	0.0 s
8	5	3	10	3.33	0.0 s
10	5	60	291	4.85	0.1 s
12	5	7848	24306	3.10	2.3 s
14	5	3459383	9503164	2.75	18 min 3 s
16	5	2585136675	6834826727	2.64	9 d 6 h
7	6	1	1	1.00	0.0 s
8	6	1	1	1.00	0.0 s
9	6	4	18	4.50	0.0 s
10	6	21	159	7.57	0.0 s
11	6	266	1407	5.29	0.1 s
12	6	7849	26416	3.37	2.8 s
13	6	367860	1018030	2.77	2 min 13 s
14	6	21609300	55550457	2.57	2 h 8 min
15	6	1470293675	3668827079	2.50	6 d 4 h

TABLE II. Connected regular graphs with girth at least 4.

n	$k = 4$	$k = 5$	$k = 6$	$k = 7$
8	1	0	0	0
9	0	0	0	0
10	2	1	0	0
11	2	0	0	0
12	12	1	1	0
13	31	0	0	0
14	220	7	1	1
15	1606	0	1	0
16	16828	388	9	1
17	193900	0	6	0
18	2452818	406824	267	8

Proof. By $r \geq i+1$, we have $\tilde{\Gamma} = \{e_1, \ldots, e_i, e_{i+1}, \ldots, e_r, \tilde{e}_{r+1}, \ldots, \tilde{e}_s\}$. Further $\tilde{\Gamma}^\pi = \{e_1^\pi, \ldots, e_r^\pi, \tilde{e}_{r+1}^\pi, \ldots, \tilde{e}_s^\pi\} \supseteq \{e_{j_1}^\pi, \ldots, e_{j_{i+1}}^\pi\} = \{e_1, \ldots, e_i, e'_{i+1}\} \Rightarrow \tilde{\Gamma}^\pi < \tilde{\Gamma}$ by $e'_{i+1} < e_{i+1}$. ∎

This means: If a nonminimal candidate was tested, determine r as in the lemma above and return to the last stage of the backtracking algorithm with $e_r \notin \Gamma$.

4. RESULTS

The introduced methods are implemented in C. The program *genreg* is designed for UNIX machines, but also runs on PCs with DOS or WINDOWS. A manual for the program, the source code, and the executables are available via http://www.mathe2.uni-bayreuth.de/markus/reggraphs.html. From this site you can even download various lists and some drawings of regular graphs.

TABLE III. Connected regular graphs with girth at least 6.

n	$k = 4$
26	1
27	0
28	1
29	0
30	4
31	0
32	19
33	0
34	1272

TABLE IV. Connected regular graphs with girth at least 5.

n	$k = 4$	$k = 5$
17	0	0
18	0	0
19	1	0
20	2	0
21	8	0
22	131	0
23	3917	0
24	123859	0
25	4131991	0
26		0
28		0
30		4

Table 1 shows results of the program for runs with given number n of vertices and degree k. It contains the number of computed regular graphs, the total number of candidates for the minimality test, the quotient of these two numbers, and the CPU-times for computation on a PC Pentium Pro with 200 MHz. Some numbers were formerly unpublished and the content exceeds similar tables as, e.g., in [4].

Results for the cases with prescribed girth larger than 3 and numbers of bipartite regular graphs are collected in Tables 2–5. In these tables no CPU-times are given, because some of the computations were done in several runs on different machines. Blanks in the tables mean that the corresponding numbers are not yet known. Numbers of cubic graphs can be found in [1].

The smallest k-regular graphs with girth g are called (k, g)-cages. The (5, 5)-cages have 30 vertices and there exist exactly four of them (see Table 4). This was first claimed by Yang and Zhang [16] in 1989. The construction of these four graphs takes 41 minutes on the PC described above. The upper left of the (5, 5)-cages in Fig. 2 is

TABLE V. Connected bipartite regular graphs.

n	$k = 4$	$k = 5$
8	1	0
10	1	1
12	4	1
14	14	4
16	129	41
18	1980	1981
20	62611	304495
22	2806490	

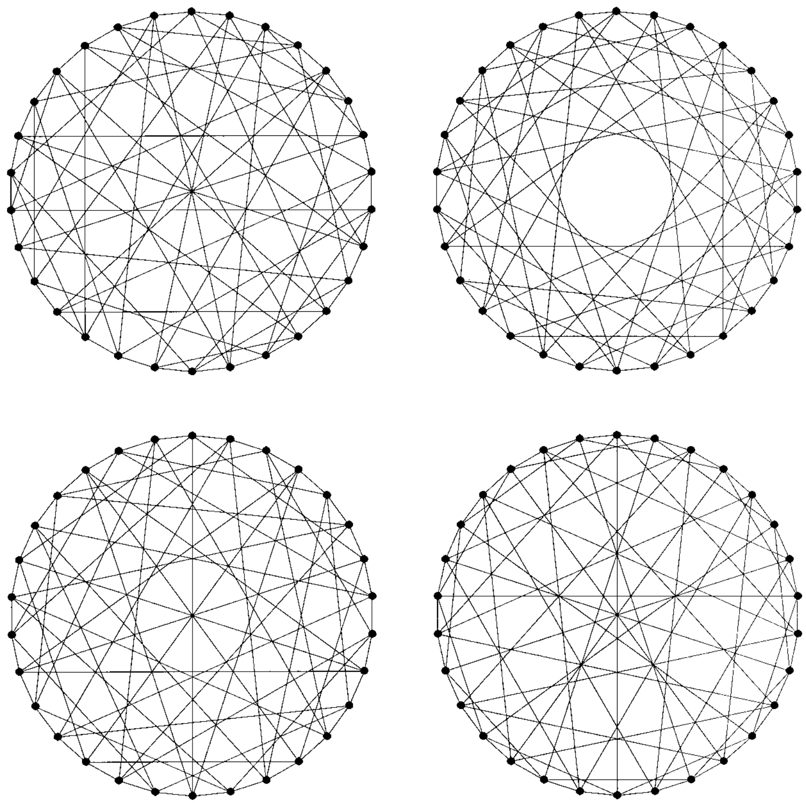

FIGURE 2. The four (5, 5)-cages.

neither mentioned in [15] nor in [3]. It has an automorphism group of order 96 and two orbits of length 6 and 24. The other (5, 5)-cages (upper right/lower left/lower right) have automorphism groups of order 30/20/120 and 2/4/2 orbits of length 15, 15/5, 5, 10, 10/10, 20. Further information can be found in Gordon Royle's catalog of cages at http://www.cs.uwa.edu.au:80/gordon/cages/allcages.html.

It turns out that graph generators like the one introduced are an important tool to confirm or disprove graph-theoretical conjectures (cf. [2], [17]). Everyone who has an open question on regular graphs is encouraged to contact the author in order to decide whether the solution is in reach of the generator.

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