

## Snakes, coils, and single-track circuit codes with spread $k$

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**Abstract** The snake-in-the-box problem is concerned with finding a longest induced path in a hypercube  $Q_n$ . Similarly, the coil-in-the-box problem is concerned with finding a longest induced cycle in  $Q_n$ . We consider a generalization of these problems that considers paths and cycles where each pair of vertices at distance at least  $k$  in the path or cycle are also at distance at least  $k$  in  $Q_n$ . We call these paths  $k$ -snakes and the cycles  $k$ -coils. The  $k$ -coils have also been called circuit codes. By optimizing an exhaustive search algorithm, we find 13 new longest  $k$ -coils, 21 new longest  $k$ -snakes and verify that some of them are optimal. By optimizing an algorithm by Paterson and Tuliani to find single-track circuit codes, we additionally find another 8 new longest  $k$ -coils. Using these  $k$ -coils with some basic backtracking, we find 18 new longest  $k$ -snakes.

**Keywords** snake, coil, circuit code, single-track, snake-in-the-box, longest path

### 1 Introduction

The *snake-in-the-box* and *coil-in-the-box* problems present difficult challenges to mathematicians and computer scientists regarding the longest induced paths or cycles in a hypercube that can be found. These problems have been heavily studied over the past 50 years [23, 9, 36, 14, 27, 44, 33, 28, 3, 41, 34, 40, 5, 42, 34, 6, 22, 12, 20, 31, 8, 10, 13, 17, 21, 26, 25, 30, 35, 39, 49, 7, 48, 4, 46, 24, 45, 37] including many dedicated to improving bounds [11, 1, 43, 2, 38, 15, 47, 16, 29]. They were first described by Kautz [23] in relation to a theory of error correcting codes, but since have appeared in many other applications including electrical engineering, coding theory, combination locking, analog-to-digital conversion and network topology. Generally, the longer the snake or coil, the more useful it is [27] while the greater the spread, the greater the error detection capability [19]. Finding the longest induced paths, however, is well known to be NP-complete even when graphs are bipartite [18].

The  $n$ -dimensional hypercube, denoted  $Q_n$ , is the graph whose vertices consist of all binary strings  $b_n \cdots b_2 b_1$  where two vertices are adjacent if and only if their binary strings differ by a single bit. An *induced path* in an undirected graph  $G$  is a path where every pair of non-consecutive vertices in the path are non-adjacent in  $G$ . Induced paths are sometimes called *snakes* and the problem of finding the longest snakes in  $Q_n$  is known as the *snake-in-the-box* problem.

A generalization of this problem is to find the longest  $k$ -snake in  $Q_n$ . A  $k$ -snake is defined to be a path in a graph  $G$  such that every pair of vertices at distance at least  $k$  in the path are also at distance at least  $k$  in  $G$ . Thus a 1-snake is a simple path and a 2-snake is an induced path. Similar problems and definitions apply for cycles. The *coil-in-the-box* problem is the problem of finding the longest induced cycles in  $Q_n$ . The more general problem is to find the optimal  $k$ -coils in  $Q_n$ . A  $k$ -coil is defined to be a cycle in a graph  $G$  such that every pair of vertices at distance at least  $k$  in the cycle are also at distance at least  $k$  in  $G$ . A 1-coil is a simple cycle and a 2-coil is an induced cycle. The parameter  $k$  is referred to as the *spread*.

The problem of finding long  $k$ -coils in  $Q_n$  was first considered by Singleton [36] using explicit constructions. Subsequently, Klee [26, 25] studied the topic using the term *circuit codes* in place of  $k$ -coils. Since then, the lower bounds for  $k$ -coils have been improved by Deimer [10], Paterson and Tuliani [31], Hiltgen and Paterson [20],

$n$	$k$					
	2	3	4	5	6	7
3	6*	6*	6*	6*	6*	6*
4	8*	8*	8*	8*	8*	8*
5	14*	10*	10*	10*	10*	10*
6	26*	16*	12*	12*	12*	12*
7	48*	24*	14*	14*	14*	14*
8	96	36*	22*	16*	16*	16*
9	188	64 <sup>a</sup> (58)	30*	24*	18*	18*
10	348	102 <sup>a</sup> (100)	46**	28*	20*	20*
11	640	160	70 <sup>a</sup> (68)	40**	30*	22*
12	1238	288	102 <sup>a</sup> (98)	60 <sup>a</sup> (58)	36**	32*
13	2468	494 <sup>b</sup> (442)	182	80 <sup>a</sup> (78)	50**	36*
14	4934	812 <sup>b</sup> (700)	280	106 <sup>a</sup> (102)	68 <sup>a</sup> (66)	48**
15	9868	1380 <sup>b</sup> (1290)	480 <sup>b</sup> (450)	210	88 <sup>a</sup> (82)	60 <sup>a</sup> (58)
16	19740	2240 <sup>b</sup> (2176)	768 <sup>b</sup> (672)	288	118 <sup>a</sup> (106)	76 <sup>a</sup> (72)
17	39840	3910 <sup>b</sup> (3842)	1224 <sup>b</sup> (1088)	476	204	102 <sup>a</sup> (90)

\* value previously known to be optimal

\*\* newly verified to be optimal

<sup>a</sup> found by partial exhaustive search

<sup>b</sup> found by optimized implementation of construction from [31]

**Table 1** Longest known  $k$ -coils. The numbers in parentheses represent best previously known values.

Zinvoik et. al [49], and Chebiryak and Kroening [7]. In [20], applications for  $k$ -coils (circuit codes) are clearly described. To the best of our knowledge, the  $n$ -dimensional hypercubes are the only class of graphs for which the  $k$ -snake and  $k$ -coil problems have been studied.

In this paper we present two algorithms that exhaustively search for long  $k$ -snakes and  $k$ -coils in  $Q_n$ . The first is an adaptation of Kochut's [28] algorithm for  $k=2$  which requires several non-trivial changes for general  $k$ , especially in the case of  $k$ -coils. At each recursive step it requires  $O(n^{k-1})$  time to update data structures. The second algorithm requires  $O(t)$  time at each recursive call, where  $t$  is the current length of the  $k$ -snake being searched. The latter algorithm is much more efficient for some small values of  $n$  and larger values of  $k$ . For  $k$ -coils, we consider two optimization strategies: the first considers a connectivity constraint and the second takes advantage of rotational equivalence. For rotational equivalence, several heuristics are considered with varying amounts of overhead. Using the best of our optimization strategies we were able to find 13 new longest  $k$ -coils and 21 new longest  $k$ -snakes. We also were able to verify that a number of previously known longest  $k$ -coils and  $k$ -snakes are indeed optimal. Since many heuristic based search algorithms in some way depend on an exhaustive search, the ideas here may provide improvements to previously studied heuristic algorithms [41, 5, 6, 12, 33, 3, 24, 4].

In addition to exhaustive search, we also applied some optimizations to a *single-track circuit code* construction algorithm by Paterson and Tuliani [31]. This allowed us to find an additional 8 longest known  $k$ -coils. Using these longest  $k$ -coils, we applied some basic backtracking to find 18 new longest  $k$ -snakes. Table 1 provides the lengths of the longest known  $k$ -coils and Table 2 provides the lengths for the longest known  $k$ -snakes. Since there has been less reporting on  $k$ -snakes, many of the previously best known bounds are obtained by removing  $k-1$  consecutive nodes from a longest corresponding  $k$ -coil. This results in a reduction of  $k$  in the length of the  $k$ -snake compared to the  $k$ -coil. The previous best known results were accumulated from [31, 49, 7, 32, 24, 45].

The remainder of the paper is outlined as follows. In Section 2 we outline two search algorithms with a comparative analysis. In Section 3 we outline a variety of optimizations for  $k$ -coils and provide an experimental analysis. In Section 4 we introduce single-track circuit codes and include an updated table of the longest known such codes. A summary is provided in Section 5. Instances of our new longest  $k$ -coils and  $k$ -snakes are provided in the Appendix. All of our searches and experiments were performed using SHARCNET<sup>1</sup>.

<sup>1</sup> This work was made possible by the facilities of the Shared Hierarchical Academic Research Computing Network (SHARC-NET:www.sharcnet.ca) and Compute/Calcul Canada.

$n$	$k$					
	2	3	4	5	6	7
3	4*	3*	3*	3*	3*	3*
4	7*	5*	4*	4*	4*	4*
5	13*	7*	6*	5*	5*	5*
6	26*	13*	8*	7*	6*	6*
7	50*	21*	11*	9*	8*	7*
8	98	35** (33)	19*	11*	10*	9*
9	190	63 <sup>a</sup> (53)	28** (26)	19*	12*	11*
10	370	103 <sup>b</sup> (83)	47** (42)	25** (23)	15*	13*
11	695	157 <sup>b</sup> (151)	68 <sup>a</sup> (64)	39** (35)	25** (24)	15*
12	1274	286 <sup>b</sup> (285)	104 <sup>a</sup> (94)	56 <sup>a</sup> (51)	33** (30)	25*
13	2466	493 <sup>b</sup> (439)	181 <sup>b</sup> (178)	79 <sup>a</sup> (73)	47 <sup>a</sup> (44)	31** (29)
14	4932	811 <sup>b</sup> (697)	279 <sup>b</sup> (276)	112 <sup>a</sup> (97)	66 <sup>a</sup> (60)	42 <sup>a</sup> (41)
15	9866	1379 <sup>b</sup> (1287)	480 <sup>b</sup> (446)	206 <sup>b</sup> (205)	89 <sup>a</sup> (76)	55 <sup>a</sup> (51)
16	19738	2240 <sup>b</sup> (2173)	766 <sup>b</sup> (668)	285 <sup>b</sup> (283)	117 <sup>a</sup> (100)	72 <sup>a</sup> (65)
17	39838	3941 <sup>b</sup> (3839)	1223 <sup>b</sup> (1084)	473 <sup>b</sup> (471)	200 <sup>b</sup> (198)	98 <sup>b</sup> (83)

\* value previously known to be optimal

\*\* newly verified to be optimal

<sup>a</sup> found by partial exhaustive search

<sup>b</sup> found by starting from a longest known coil and backtracking

**Table 2** Longest known  $k$ -snakes. The numbers in parentheses represent best previously known values.

## 2 Exhaustive search algorithms

Kochut's algorithm [28] that exhaustively searches for optimal 2-snakes follows a straightforward recursive backtracking approach with one key optimization: it takes advantage of the symmetry of  $Q_n$  to assume that every snake starts at  $0^n$  and each dimension  $d$  is visited before any dimension greater than  $d$  (i.e., it considers equivalence under permutation of the bit positions). Thus, the following 3 snakes are equivalent with the first being the canonical form searched by the algorithm:

$$[0000, 0001, 0011, 0111, 0110], \quad [0000, 1000, 1010, 1110, 0110], \quad [1111, 0111, 0101, 0001, 1001].$$

In the next two subsections we outline two approaches that apply this optimization. In the final subsection we provide a comparative analysis. To simplify our discussion, we say that a vertex  $y$  *conflicts* with vertex  $x$  if the two vertices differ in fewer than  $k$  bit positions.

### 2.1 Approach one: Search( $t, d$ )

The first search method we discuss follows the standard exhaustive search approach used for  $k = 2$ . The basic idea is to update the conflicts with unused vertices as the search path gets extended. This allows a constant time test to determine whether or not a search path can be extended through a given vertex  $x$ . The data structure required to maintain the conflicts is an array  $numConflicts$  where each  $numConflicts[x]$  stores the number of vertices in the current search path  $\alpha$  that are in conflict with  $x$ . Since each vertex is in conflict with  $c = \binom{n}{1} + \binom{n}{2} + \dots + \binom{n}{k-1}$  other vertices in  $Q_n$ , updating  $numConflicts$  will require  $O(c) = O(n^{k-1})$  time every time a vertex is added to the path.

Pseudocode for such a recursive  $k$ -snake and  $k$ -coil search algorithm in  $Q_n$  is illustrated by the function  $Search(t, d)$  in Figure 1. The  $k$ -snake ( $k$ -coil) being searched at the start of each recursive call is stored in  $\alpha = a_0 \dots a_{t-1}$ , where each  $a_i$  is the integer representation of vertex  $i$ . The parameter  $t$  indicates the length of the current path and  $d$  indicates the largest dimension currently visited. The other global variables used are:

- $numConflicts[x]$ : the number of vertices in  $\alpha$  that conflict with  $x$ ,
- $adj[x][d]$ : the neighbor of  $x$  obtained by flipping the  $d$ -th bit,
- $conflict[x]$ : the set of  $c$  vertices in  $Q_n$  that conflict with  $x$ ,

Note that the arrays  $adj$  and  $conflict$  are easily pre-computed. To run the algorithm, we initialize  $numConflicts[x] = 0$  for each vertex  $x$  and then set the first  $k + 1$  vertices in the path to  $0, 2^1 - 1, \dots, 2^k - 1$ , incrementing

```

procedure Search( $t, d$ : int)
int  $i, x, y$ 
1: for  $i$  from 1 to Min( $d + 1, n$ ) do
2:    $x := a_t := adj[a_{t-1}][i]$ 
3:   if numConflicts[ $x$ ] <  $k$  then
4:     for each  $y \in conflict[x]$  do numConflicts[ $y$ ]++
5:     CheckMaximal( $t$ )
6:     Search( $t + 1, \text{Max}(i, d)$ )
7:     for each  $y \in conflict[x]$  do numConflicts[ $y$ ]--

```

**Fig. 1** Exhaustive search algorithm for optimal  $k$ -snakes or  $k$ -coils in  $Q_n$ .

```

function CheckMaximal( $t$ : int) returns boolean
int  $x$ 
1: if bits[ $a_t$ ] >  $k$  or maxlen  $\geq t + k$  then return FALSE
2: if bits[ $a_t$ ] = 1 then
3:   Print( $a_0 \cdots a_t$ )
4:   maxlen :=  $t + 1$ 
5:   return TRUE
6: for each  $x \in adjSmaller[a_t]$  do
7:    $a_{t+1} := x$ 
8:   if numConflicts[ $x$ ] =  $k$  and CheckMaximal( $t + 1$ ) then return TRUE
9: return FALSE

```

**Fig. 2** Recursive function to check if an initial search path  $a_0 \cdots a_t$  can be extended to a  $k$ -coil.

the conflicts for each vertex. The initial recursive call is  $\text{Search}(k + 1, k)$ . During a recursive call, each neighbor  $x$  of the last vertex  $a_{t-1}$  is checked to see if it extends the path without violating the constraints on  $k$  or  $d$ . In order to abide by the constraint on  $k$ , there can be at most  $k - 1$  vertices (the last  $k - 1$  vertices) that conflict with  $x$ . If  $x$  does not violate the constraints, we increment  $\text{numConflicts}[y]$  for each vertex  $y$  that conflicts with  $x$  and then recursively look for longer  $k$ -snakes.

If we are interested in generating  $k$ -snakes, the function  $\text{CheckMaximal}(t)$  will check if  $a_0 \cdots a_t$  is the longest  $k$ -snake found so far. By maintaining the variable  $\text{maxlen}$  to represent the longest  $k$ -snake found in the search, a new longest  $k$ -snake will be found if  $\text{maxlen} < t$ . For  $k$ -coils, the test is more complicated because the search algorithm will never visit vertices with fewer than  $k$  bits after the initialization steps. Thus when  $a_t$  has exactly  $k$  bits set to 1 and  $\text{maxlen} < t + k$ , we perform a special test to see if there is a valid direct path from  $a_t$  to  $a_0$ .

To efficiently perform the  $k$ -coil test, we pre-compute two additional data structures. First, we let  $\text{bits}[x]$  store the number of bits set to 1 in the binary representation of  $x$ . Second, we let  $\text{adjSmaller}[x]$  be a set of the  $\text{bits}[x]$  vertices that are neighbors of  $x$  and have one fewer bit set to 1. Using these data structures, the function  $\text{CheckMaximal}(t)$  shown in Figure 2 recursively checks if a direct path exists back to the starting vertex  $a_0$ . Observe that for each recursive call, each neighbor of  $a_t$  with one fewer bit set to 1 can be visited efficiently using  $\text{adjSmaller}[a_t]$ , extending the  $k$ -coil one step closer to the start vertex 0. Note that each vertex in the return path will conflict with exactly  $k$  vertices in the original search path  $a_0 \cdots a_t$  being tested. For instance, if  $k = 4$  the vertex  $a_{t+1}$  (in the original recursive call) will have  $k - 1$  bits set to 1. It will be distance 1 from  $a_{t-1}$ , distance 2 from  $a_{t-2}$ , distance 3 from  $a_{t-3}$  and also distance 3 from  $a_0$ , but a distance of at least  $k$  from all other vertices in  $\alpha$ . In the base case when the last vertex is adjacent to 0 (it will have one bit set to 1), we update  $\text{maxlen}$  and print out the  $k$ -coil.

In the worst case, if no such path is found, the function  $\text{CheckMaximal}(t)$  for  $k$ -coils will run independently of  $n$  in  $O(k!)$  time. However, since the recursive check is rarely required, the running time of this function has little impact on the overall search time. As an example, in the case of  $n = 6$  and  $k = 2$  there are a total of 651075 recursive search calls, but the  $O(k!)$  recursive check is only performed 22 times. Since  $\text{CheckMaximal}(t)$  is very efficient for both  $k$ -snakes and  $k$ -coils, the  $O(e) = O(n^{k-1})$  update of the conflicts dominates the running time of  $\text{Search}(t, d)$ .

Note that the space required by this algorithm is  $O(n^{k-1}2^n)$ . This is the space needed to store the array  $\text{conflict}$ . This can be reduced to  $O(2^n)$  if both the conflicts and the adjacencies are computed on demand. Each of these operations can be done efficiently using bitwise operations on integers.

```

function IsConflict( $t, s$ : int) returns boolean
int  $j$ 
1: for  $j$  from  $t - k - 1$  down to  $s$  do
2:   if  $inConflict[a[t]][a[j]]$  then return TRUE
3: return FALSE

procedure Search2( $t, d$ : int)
int  $i$ 
1: for  $i$  from 1 to  $\text{Min}(d + 1, n)$  do
2:    $a_t := adj[a_{t-1}][i]$ 
3:   if not IsConflict( $t, 0$ ) then
4:     CheckMaximal( $t$ )
5:     Search2( $t + 1, \text{Max}(i, d)$ )

```

**Fig. 3** Alternate search algorithm for  $k$ -snakes and  $k$ -coils in  $Q_n$ .

## 2.2 Approach two: Search2( $t, d$ )

For  $k = 2$  the time required to update conflicts in  $\text{Search}(t, d)$  is an efficient  $O(n)$ , however as  $k$  gets bigger the overhead for the updates can be significantly larger than the length of an optimal  $k$ -snake or  $k$ -coil. For instance, when  $n = 10$  and  $k = 5$  each vertex has 385 conflicts. Thus adding a vertex to a search path requires executing two **for** loops iterating 385 times each. The updates are performed so it is possible to test whether a vertex  $x$  can extend the current search path in constant time. As an alternative, the following method to check conflicts will be more efficient in some cases: test  $x$  for a conflict with each vertex in the current search path not including the last  $k - 1$  vertices. In fact, when considering adding  $x = a_t$  to the search path  $a_0 \cdots a_{t-1}$ , we need only see if  $x$  is in conflict with any of the vertices in  $a_0 \cdots a_{t-k-1}$ , since if  $x$  is in conflict with  $a_{t-k}$ , it will also be in conflict with  $a_{t-k-1}$ . During each recursive call, testing for these conflicts must be done for each of the  $n$  neighbors of  $a_{t-1}$ . Observe that exactly  $k$  of these neighbors will be in conflict with  $a_{t-k-1}$ . The remaining  $n - k$  neighbors that are not in conflict with  $a_{t-k-1}$  will require  $t - k$  comparisons to test for conflicts in the worst case. Therefore, using this alternate approach, in the worst case each recursive call will require  $(n - k)(t - k) + k$  comparisons. When  $n = 10$  and  $k = 5$ , the longest  $k$ -snake is 25, so the worst case will only require  $5 \cdot 20 + 5 = 105$  comparisons. This is a significant improvement over the 770 loop iterations required by  $\text{Search}(t, d)$ .

Pseudocode for this alternate approach,  $\text{Search2}(t, d)$  is given in Figure 3. It requires the same initialization as  $\text{Search}(t, d)$ . The function  $\text{IsConflict}(t, s)$  tests whether or not  $a_t$  is in conflict with any vertex in  $a_{t-k-1} \cdots a_s$ . It assumes that the  $conflict[x][y]$  is precomputed to store a 1 if the  $x$  conflicts with  $y$  and store a 0 otherwise. Because the array  $numConflicts$  is no longer maintained, the function  $\text{CheckMaximal}(t)$  requires a more expensive test for conflicts as well. Specifically, a vertex will be in conflict if  $\text{IsConflict}(t + 1, k - bits[a[t]] + 1)$  returns TRUE. However, since this test is so rarely required, it will have an insignificant impact on the search time.

Note that the space required by this algorithm is  $O(4^n)$  to store the values in the 2-dimensional array  $inConflict$ . If testing for a conflict between two vertices is done on demand and the adjacencies are also computed on demand (each of these operations can be done efficiently using bitwise operations on integers), then the space requirement can be reduced to  $O(s)$  where  $s$  is a bound on the maximum length of the snake or coil that can be generated.

## 2.3 Comparing algorithms

We compare the running times (measured in seconds) of the two approaches for some values of  $n$  and  $k$  in the following table.

$(n, k)$	(7,2)	(8,3)	(9,4)	(10,5)	(11,5)	(12,6)
<b>Search</b>	680210	137	5.04	1.02	23606	2009
<b>Search2</b>	2334000	214	2.93	0.26	5464	168

While difficult to prove, it is reasonable to assume that for each  $k$ , there is an integer  $m$  such that for all  $n < m$ ,  $\text{Search2}$  will be faster than  $\text{Search}$ , and that for all  $n \geq m$ , the first approach will be faster. To illustrate this further, we compare the number of updates to the array  $numConflicts$  required to generate each recursive call to

Search with the worst case number of comparisons required to determine conflicts during each recursive call to Search2. Recall that these two values are represented by  $2c = 2(\binom{n}{1} + \binom{n}{2} + \dots + \binom{n}{k-1})$  and  $(n-k)(s-k) + k$ , where  $s$  represents the longest known  $k$ -snake of length  $n$ .

$(n, k)$	(6,3)	(7,3)	(8,3)	(10,4)	(11,4)	(12,4)	(12,5)	(13,5)	(14,5)
$2c$	42	56	72	350	462	596	1586	1984	2540
$(n-k)(s-k)+k$	33	75	163	262	452	804	362	597	914

For  $k = 2$ , Search always has fewer comparisons than Search2 (this is easy to verify). For  $k = 3$ , Search2 has fewer comparisons when  $n \leq 6$ . For  $k = 4$ , Search2 has fewer comparisons for all  $n < 12$ . For  $n = 12$ , it is hard to evaluate because even though  $804 > 596$ , the value for 804 is worst case and not average case. For  $k = 5$  it is clear that Search2 has fewer comparisons for  $n \leq 14$ .

### 3 Optimizations for $k$ -coils

In the next two subsections, two approaches that attempt to optimize the search algorithm for  $k$ -coils will be discussed. The first approach considers connectivity and the second approach considers rotational equivalence. Recall that the number of bits set to 1 for each vertex  $v$  is pre-computed in  $bits[v]$ .

#### 3.1 Connectivity

In this subsection we consider a simple connectivity property when searching for optimal  $k$ -coils. In particular, given a  $k$ -snake  $\alpha = a_0 \dots a_t$  in  $Q_n$ , if we know that it is impossible to extend  $\alpha$  into a  $k$ -coil, then we can terminate this search branch of the computation tree. Unfortunately, a complete test for connectivity does not seem practical since even an  $O(2^n)$  breadth-first-search is not sufficient. Thus, we discuss a simplified but efficient test that can be used to detect some of these dead ends.

Consider a partition of the vertices into  $n+1$  subsets  $V_0 \dots V_n$  such that each subset  $V_i$  contains the  $\binom{n}{i}$  bitstrings with  $i$  bits set to 1. The basic idea of our approach is as follows: if a vertex from  $V_i$  is appended to the current  $k$ -snake so that for some  $j < i$  no vertex in  $V_j$  can be reached without violating the conflict constraint, then it is impossible to return to  $a_0 = 0$ . For example, consider the  $k$ -snake  $[0, 1, 3, 7, 6, 14, 12, 28, 24, 56, 48, 52]$  for  $n = 6$  and  $k = 2$  using integer representations for the vertices. The subset  $V_1 = \{1, 2, 4, 8, 16, 32\}$  has no available vertices since 3 is adjacent to 1 and 2, 12 is adjacent to 4 and 8, and 48 is adjacent to 16 and 32. Thus using the partial connectivity test we can terminate this search branch of a  $k$ -snake at length 11, which is considerably shorter than the optimal  $k$ -coil of length 26.

It is possible to efficiently implement this optimization in  $O(n^{k-1} + k^2)$  time in the worst case which is comparable to the time required to update the array  $numConflicts$  using  $Search(t, d)$ . Thus the extra work only increases the complexity by a constant factor per recursive call. However, because the extra work almost doubles the computation required at each recursive call, it is important to reduce the number of recursive calls by a significant factor for this optimization to be useful. We illustrate the effect of this optimization with respect to the number of recursive calls required for some small values of  $n$  and  $k$  in the following table:

$(n, k)$	(6,2)	(7,3)	(8,3)	(8,4)	(9,4)	(9,5)	(10,5)
<b>Non-optimized</b>	651075	26060	556120186	4624	7817954	1963	557993
<b>Connectivity</b>	389257	15719	300717441	2424	3840003	1345	277788
<b>% Reduction</b>	40	40	46	48	51	31	50

It does not appear that this optimization leads to significant savings in run-time. In fact, for each of the experiments, the optimized version actually requires slightly more time. One reason why this heuristic does not appear to be effective may be because most of the dead ends found occur deep in the recursion.

#### 3.2 Rotational equivalence

Since  $k$ -coils are cycles it is natural to consider equivalence under rotation. For example, consider the 2-coil of length 8 illustrated in Figure 4. Depending on which of the 8 vertices is the starting vertex, up to 8 different

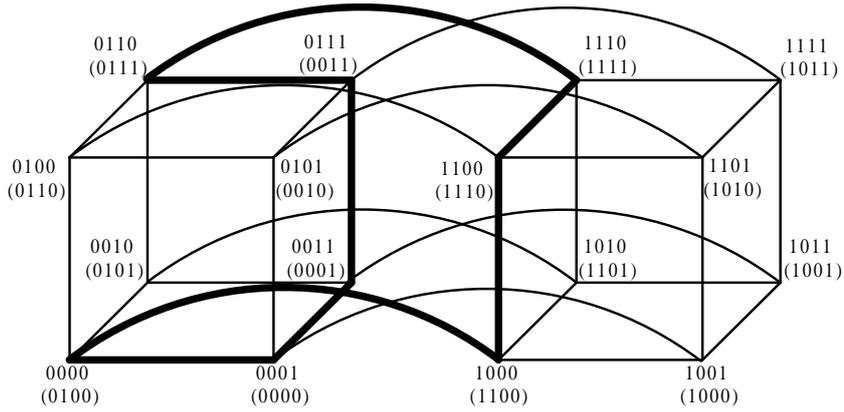


Fig. 4 Illustration of two rotationally equivalent 2-coil sequences in  $Q_4$ .

equivalent vertex sequences can be obtained, even when the vertices are relabel so they match the canonical form outlined earlier: label the first vertex  $0^n$  and visit dimension  $d$  before  $d + 1$ . The two different, but equivalent 2-coils illustrated in this figure are:

$$\begin{aligned} & [0000, 0001, 0011, 0111, 0110, 1110, 1100, 1000], \\ & [0000, 0001, 0011, 0111, 1111, 1110, 1100, 0100]. \end{aligned}$$

In this subsection we explore four different methods for testing for partial rotational equivalence. For a given rotational test, we say a search path  $\alpha$  is a *dead end* if it is not in a specified canonical form. We use the term *canonical* loosely, since the tests are only partial tests and equivalent  $k$ -coils may be generated from different canonical branches. In one of the tests, we also take advantage of equivalence under reversal. However, in general, this is an expensive test for at best an additional 50% reduction in the search space.

We visit the four methods in order of time complexity per recursive call to perform the rotational test. Each optimization is independent of which search algorithm it is applied to: **Search** or **Search2**. They can be summarized as follows:

- ▷ diagonal  $O(1)$ ,
- ▷ pre-diagonal  $O(n)$ ,
- ▷ pre-diagonal w/reversal  $O(n)$ ,
- ▷ bit count sequence  $O(t) = O(\text{snakelength})$ .

In Section 3.2.5, we provide an analysis comparing the impact on the number of recursive calls and the overall run time for feasible values of  $n$  and  $k$ .

### 3.2.1 The diagonal

The first method can be implemented very simply and efficiently. We say that two vertices are *diagonal* to each other in  $Q_n$  if the two vertices are complements to each other, i.e., their integer representations sum to  $2^n - 1$ . If two vertices  $a_i$  and  $a_j$  are diagonal to each other in a search path  $\alpha$  where  $i < j$ , then the *length* of the diagonal is given by  $j - i$ ; if one of the vertices is not in the path then the length of their diagonal is  $2^n$ . If we let  $len$  denote the length of the diagonal between  $a_0 = 0$  and its complement, then we say a search path  $\alpha$  is in a canonical form if every diagonal has length at least  $len$ . For example when  $n = 6$  and  $k = 2$ , consider the following search path  $\alpha$  where the vertices are represented by integers:  $[0, 1, 3, 7, 6, 14, 12, 13, 29, 31, 63, 55, 51]$ . Since  $len = 10$  and the diagonal between 12 and 51 has length 6, this path is not in a canonical form. Thus  $\alpha$  is a dead end.

The following steps can be used to efficiently implement this optimization:

1. Maintain the global variable  $len$  to store the length of the diagonal between  $0^n$  and  $1^n$ .
2. Maintain the global array  $pos$  where  $pos[v]$  is the index of the vertex  $v$  in  $\alpha$  (or  $-2^n$  if not in  $\alpha$ ).
3. Detect a dead end if  $t - pos[2^n - 1 - a_t] < len$ .

Observe that these modifications can easily be applied in  $O(1)$  time per recursive call.

### 3.2.2 The pre-diagonal

In an attempt to remove more isomorphic branches of the exhaustive search, we consider a slightly more expensive test for equivalence. A vertex  $x$  is said to be *pre-diagonal* to a vertex  $y$  if the two vertices differ in  $n-1$  bit positions. Thus each vertex will have  $n$  vertices that are pre-diagonal to it. For example, the 5 pre-diagonals to 00000 are 01111, 10111, 11011, 11101, 11110. If  $a_i$  and  $a_j$  are pre-diagonal to each other in a path  $\alpha$  where  $i < j$ , then the length of the pre-diagonal is  $j - i$ . Now, similar to our diagonal test, by focusing on the length of all pre-diagonals in a search path we can obtain a canonical form. If  $len$  denotes the length of the shortest pre-diagonal including  $0^n$ , then we say a search path  $\alpha$  is in a canonical form if every pre-diagonal has length at least  $len$ . If there is no pre-diagonal with  $0^n$ , then  $len = 2^n$ . For example, if  $n = 6$  and  $k = 2$ , the search path [0, 1, 3, 7, 15, 13, 29, 61] is a dead end since the shortest pre-diagonal with 0 is 61 (111101) at length 7 while the length between 3 (000011) and 61 (111101) is 5. Similarly, the search path [0, 1, 3, 7, 6, 14, 30] is a dead end since 1 (000001) and 30 (011110) are pre-diagonals but there is no pre-diagonal with 0.

The following steps can be used to efficiently implement this optimization:

1. Pre-compute the set  $pdlist[v]$  for each vertex  $v$  that contains the  $n$  vertices that are pre-diagonal to  $v$ .
2. Maintain the global variable  $len$  to store the length of the shortest pre-diagonal with  $0^n$ .
3. Maintain the global array  $pos$  where  $pos[v]$  is the index of the vertex  $v$  in  $\alpha$  (or  $-2^n$  if not in  $\alpha$ ).
4. Detect a dead end if  $t - pos[v] < len$  for any  $v \in pdlist[a_t]$ .

Detecting a dead end requires  $O(n)$  time in the worst case and the other variables are easily maintained in  $O(1)$  time. Thus, these modifications can easily be applied in  $O(n)$  time per recursive call.

### 3.2.3 Refined pre-diagonal with reversal

The pre-diagonal test still allows equivalent search paths where there are multiple pre-diagonals of length  $len$ . To remove even more equivalent branches of computation we refine our definition of a canonical search path by considering the second longest pre-diagonals from each vertex. Let  $len2$  denote the second longest pre-diagonal containing 0. If no such pre-diagonal exists then  $len2 = 2^n$ . A search path is in a canonical form if (1) every pre-diagonal has length at least  $len$  and (2) if a vertex has a pre-diagonal of length  $len$  then the length of its second longest pre-diagonal must be at least  $len2$ . For example, consider the following search path where  $n = 6$  and  $k = 3$ : [0, 1, 3, 7, 15, 31, 30, 28, 60]. The only pre-diagonal with 0 is 31 with  $len = 5$ , but 1 is pre-diagonal with both 30 and 60. The lengths of these pre-diagonals are 5 and 7 respectively, so this search path is a dead end.

Since  $k$ -coils also have equivalence under reversal, we can refine our canonical form even further by enforcing this condition on the reversal. As an example with  $n = 6$  and  $k = 3$ , consider [0, 1, 3, 7, 15, 31, 29, 28, 60]. Again, the only pre-diagonal with 0 is 31 with  $len = 5$ , however 60 is pre-diagonal with both 7 and 1. The lengths in the reverse direction from 60 are 5 and 7 respectively, so this path is a dead end.

In addition to the modifications described in the previous subsection, the following steps can be used to efficiently implement this optimization:

1. Maintain the global variable  $len2$  in  $O(1)$  time.
2. Maintain the boolean array  $b$  such that  $b[v]$  is TRUE if and only if the vertex  $v$  is in the search path and has a pre-diagonal at length  $len$ .
3. Detect a dead end if for any  $v \in pdlist[a_t]$  where  $b[v] = \text{TRUE}$  we have  $t - pos[v] < len2$ .
4. Compute two boolean flags:  $f_1$  and  $f_2$ . The flag  $f_1$  is TRUE if and only if there exists a  $v \in pdlist[a_t]$  such that  $t - pos[v] = len$ . The flag  $f_2$  is TRUE if and only if there exists a  $v \in pdlist[a_t]$  such that  $len < t - pos[v] < len2$ .
5. Detect a dead end (for reversals) if both  $f_1$  and  $f_2$  are TRUE.

Maintaining the array  $b$  and setting the flags can easily be done in  $O(n)$  time. Thus, for this heuristic detecting a dead end requires at most  $O(n)$  time.

### 3.2.4 Bit count sequence

A more complete test for rotational equivalence applies a lexicographic approach to the path being searched. The bit count sequence of a search path  $\alpha = a_0 \cdots a_t$  is a sequence of the number of bits in each vertex  $a_i$  that differ from  $a_0$ . For example, recall the two equivalent 2-coils introduced earlier:

$$\begin{aligned} & [0000, 0001, 0011, 0111, 0110, 1110, 1100, 1000], \\ & [0000, 0001, 0011, 0111, 1111, 1110, 1100, 0100]. \end{aligned}$$

The bit count sequences for these 2-coils are  $\langle 0, 1, 2, 3, 2, 3, 2, 1 \rangle$  and  $\langle 0, 1, 2, 3, 4, 3, 2, 1 \rangle$  respectively. We say a search path is in canonical form if the bit count sequence starting from 0 is lexicographically largest compared to the bit count sequences starting from the other vertices in the search path. As an example, consider the search path  $\alpha$  illustrated in Figure 5. The bit count sequence is  $\langle 0, 1, 2, 3, 4, 3, 4, 3, 4, 3, 2 \rangle$ . However, the bit count sequence relative to starting at vertex 01101 is  $\langle 0, 1, 2, 3, 4, 5 \rangle$ . Since this is lexicographically larger than the bit count sequence for  $\alpha$ , the search path  $\alpha$  is not in canonical form and we detect a dead end.

$\alpha$	00000	00001	00011	00111	01111	01101	11101	11001	11011	11010	10010
00000	<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>3</b>	<b>4</b>	<b>3</b>	<b>4</b>	<b>3</b>	<b>2</b>
00001		0	1	2	3	2					
00011			0	1	2	3	4	3	2		
00111				0	1	2	3	4	3	4	3
01111					0	1	2	3	2		
<b>01101</b>						<b>0</b>	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
11101							0	1	2	3	4
11001								0	1	2	3
11011									0	1	2
11010										0	1
10010											0

**Fig. 5** A dead end search path  $\alpha$  when considering rotational equivalence using the bit count sequence.

Note that once a bit-count sequence is smaller than the bit-count sequence of  $\alpha$ , like the one starting with 00001,  $\langle 0, 1, 2, 3, 2 \rangle$ , we no longer need to consider it for rotational testing. Also, even though they are illustrated in the table, we do not need to consider the bit count sequences starting from  $a_t, a_{t-1}, \dots, a_{t-k}$ , as they will always start  $0, 1, \dots, k$ .

The following steps can be used to efficiently implement this optimization:

1. Pre-compute the Hamming distance between every pair of vertices  $u$  and  $v$  in  $\text{diff}[u][v]$ .
2. Maintain the global array  $\text{test}$ , initialized to  $2^n$ , to determine which starting positions require testing. When appending  $a_t$ , if the bit-count sequence starting from  $a_i$  becomes less than the bit-count sequence for  $\alpha$ , then  $\text{test}[i]$  gets updated to  $t$ . If  $\text{test}[i] < t$ , the bit-count sequence starting from  $a_i$  can be safely ignored.

Using the pre-computed array  $\text{diff}$  it is possible to test each bit-count sequence in constant time: the next value in the bit-count sequence relative to  $a_i$  is  $\text{diff}[a_i][a_t]$ . Thus, this optimization requires  $O(t - k)$  time.

A slight improvement can be made if we maintain a linked list that contains only the positions  $i$  that need to be tested. To maintain the linked list requires extra overhead (and code-complexity) as elements have to be removed during the test and then restored after the recursive call. However, in the amortized sense, it requires only a constant amount of extra work for each vertex in the list. In the following subsection we report experimental results with and without using such a linked list.

### 3.2.5 Experimental results

In Table 3, the number of recursive calls required by the non-optimized search algorithm is compared to the four optimized approaches utilizing rotational equivalence is considered. Generally, the more expensive the optimization, the larger the reduction in the number of recursive calls.

$(n, k)$	(6,2)	(7,3)	(8,3)	(8,4)	(9,4)	(9,5)	(10,5)
<b>Non-optimized</b>	651075	26060	556120186	4624	7817954	1963	557993
<b>Diagonal</b>	114042	13940	365822530	2329	6647281	898	442018
<b>Pre-diagonal</b>	226152	8299	85528048	1359	952904	682	92333
▷ <b>Pre-diagonal w/reversal</b>	85643	3415	47446549	802	617453	498	77030
<b>Bit count</b>	50337	2647	26620597	542	432632	372	27611

**Table 3** A comparison on the number of recursive calls required for exhaustive search on select  $k$ -coils.

It is interesting to note the impact on the number of recursive calls in case additional processing is desired by some application as each new vertex is appended to a search path. But ultimately we are interested in evaluating the impact that each optimization has on the overall running time. Such timing results are given in Table 4. The base search algorithm `Search` was used for  $(n = 7, k = 2)$  and  $(n = 8, k = 3)$ , while `Search2` was more efficient for the remaining cases. Each experiment was run on an Opteron 2.2 GHz processor. In each case, the bit count sequence implemented with a linked list was the most efficient.

$(n, k)$	(7,2)	(8,3)	(10,4)	(11,5)	(12,6)
<b>Non-optimized</b>	680210	137	1303000	5460	168
<b>Diagonal</b>	46641	92	1351000	6510	181
<b>Pre-diagonal</b>	128652	24	199800	2590	134
▷ <b>Pre-diagonal w/reversal</b>	77660	16	197700	2415	143
<b>Bit count</b>	45756	9	60800	255	7
▷ <b>Bit count w/linked list</b>	35652	8	58000	243	7

**Table 4** A comparison on the running time (in seconds) required to exhaustively search some  $k$ -coils for various values of  $n$ . `Search` was used for (7,2) and (8,3) and `Search2` was used for (10,4), (11,5), (12,6).

### 3.3 Applying the optimized algorithms

Using the optimized exhaustive search algorithm, we used SHARCNET to search for new long  $k$ -snakes and  $k$ -coils. Using 10 processors to perform the search with a limit of 7 days for each  $(n, k)$  pair, we were able to find 13 new longest  $k$ -coils, 21 new longest  $k$ -snakes. We also verified that several previously known  $k$ -snakes and  $k$ -coils were indeed optimal. These results are shown in Table 1 and Table 2. Instances of each new longest  $k$ -coil and  $k$ -snake are given in the Appendix.

## 4 Single track circuit codes

A *single-track circuit code* is a  $k$ -coil (circuit code) with an additional property: each track (the sequence of bits obtained by isolating a given bit position) is a cyclic shift of the first track. For example, consider the two 2-coils below.

0000	0000
0001	0001
0011	0011
0111	0111
1111	1111
1110	1011
1100	1010
1000	1000

The first track in the left 2-coil is the sequence of the bits from the left most bit position: 00001111. The 2nd track is 00011110, the third track is 00111100, and the 4th track is 01111000. Each of these tracks is a cyclic shift of

$n$	$k$					
	1	2	3	4	5	6
2	4*	4*	-	-	-	-
3	6*	6*	6*	-	-	-
4	8*	8*	8*	8*	-	-
5	30*	10*	10*	10*	10*	-
6	60*	24*	12*	12*	12*	12*
7	126*	42*	14*	14*	14*	14*
8	240	80	16	16*	16*	16*
9	504*	162	54	18	18*	18*
10	960	320	80	20	20*	20*
11	2046*	594	154	22	22	22*
12	3960	960	288	96	24	24
13	8190*	1898	494 (442)	182	26	26
14	16128	3528	812 (700)	280	28	28
15	32730	6630	1380 (1290)	480 (450)	210	30
16	65504	12512	2240 (2176)	768 (672)	288	32
17	131070*	22406	3910 (3842)	1224 (1088)	476	204

\* value previously known to be optimal

**Table 5** Longest known single-track circuit codes. The numbers in parentheses represent best known values previous to this research.

the first track and so the 2-coil is also a single-track circuit code. As another example, consider the 2-coil on the right. The first track is 00001111 and the second track is 00011000. Since the second track is not a cyclic shift of the first track the 2-coil does not have the single-track property. The notion of the single-track property was first introduced in [21] with a focus on circuit codes in [20].

Many of the previously known longest  $k$ -coils are due to a construction for single-track circuit codes by Paterson and Tuliani [31]. By implementing their construction with an optimization that considers equivalence under rotation, we were able to extend many of their previously reported results. In particular, we found 8 new longest single-track circuit codes for various  $n$  and  $k$  as illustrated in Table 5. Instances of these new longest single-track circuit codes are listed in the Appendix and they also represent 8 new longest  $k$ -coils. By applying backtracking to these long  $k$ -coils, we have also found many new longest known  $k$ -snakes. These new bounds are shown in Table 1 and Table 2 respectively.

## 5 Summary

By optimizing an exhaustive search algorithm, we find 13 new longest  $k$ -coils, 21 new longest  $k$ -snakes, and verify that some of them are optimal. By optimizing an algorithm by Hiltgen and Paterson [31] to find single-track circuit codes, we additionally find another 8 new longest single-track circuit codes and 8 new longest  $k$ -coils. Using these  $k$ -coils with some basic backtracking, we find 18 new longest  $k$ -snakes. Instances of each of these new longest  $k$ -coils and  $k$ -snakes are provided in the Appendix.

Future work in this area may be to apply the exhaustive search optimizations to both new and known heuristic approaches in the search for longer  $k$ -snakes and  $k$ -coils, especially when  $k > 2$ . Additionally, it would be interesting to study  $k$ -snakes and  $k$ -coils in the context of other graph classes.

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7d1a562ae78g43fe67f1283d6137fag235d8ac5ea06e405dgg43f50a7e3045328d9b08g23c5186729a08g52369e2f0143g012e41d706843bd9c27beca8bge9a21ef8adgb  
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(12.4,102): 0123456137580635209165071a630126504176081265092317b0247168249a1736259712067329876124a6531a76925a614ba

(15.4,480,000010001101101): 19a7b2e306ad748a91c30a21d5cea2dbe78590c1d48b52687ea1d80eb3ac80b9c5637daeb2693046c58eb6dc918a6d97a3415b8c9047  
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(16.4,768,0000010001001101): 14a90f23789cf6d3406c9e4dc53ad0631dbce0148f5b1d9ae176dcf04569c3a01d39661a9207ad30ea89bd15c28ea67be43a9cd1236  
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(17.4,1224,00000010010100011): 2134a80b5a31206b74g0582b10f2e5879gb10c4f256gc104f3701b865cd80b1935ge08d27689fd5gaf8675b9c945ad7g65372adce4  
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(12.5,60): 012345678239a562b9145678910a7631204567820ba5629b145678b13a7

(13.5,80): 012345671824951a640253a4b0c382401932a709b2640719cb3754192a38c12097a14230b762a3c

(14.5,106): 012345671839501234560a2b35c012345608319507329ad7062ca73125a43085942635104c36a0b423506143870c1359721ca569d

(14.6,68): 01234567829a45b702c4adb301ca9b7601892570cd12473ad82970ab68475d3a64c

(15.6,88): 012345607182930a142b35061743c085d123046915703e9ca10426bc134508a9c765421cabd76350417c8b5

(16.6,118): 012345607182930a142b35061743c085d1230469157038a1420e361f25073b12408691370d582a74019c3876dc210e67b319a246735d0a19fb75a

(16.7,76): 0123456708192a3b041c253d06172e480597bf18c4a92307c86e24b958012cea4870d62afb7

(17.7,102): 0123456708192a3b041c253d06172e48031f259406172a3b051g789dc0b324ed109ab76de2c0153be89a0124cefd3b072e95d

(15.7,60): 2e571b9ac682531946cd5e17402cb6184d9c2e1a5d8327eb1c682470bd9

### A.2 k-snakes

(8.3,35): 01230425614273614067153762541650341

(9.3,63): 012304250123062704135423041356280524032105240726531403245314072

(10.3,103): 1536123415301239156241350183612345023715361234153012391437153012341536123715381239153012341536123915302

(11.3,157): 012341563078209867a52795831503786218023942598371435190a1203984a924056415903a601a527a42059675462186a1520782a71437642158316  
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(13.3,493): 0123456705189ab147892460c4a9c579417c640c7814ca54b2063b1a2071c5916094a01ba9c159a2b19641375c83b675ab940bc50165b3609b40673b0c  
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**(11,5,39):** 012345671285970a814576a83425a9641570963

**(12,5,56):** 012345671285970a81479b5867a9218754361897a0145b9761428b71

**(13,5,79):** 01234506172850913254061a2b03172c045b239654013894ba136709435a6c29173ca897064a8b5

**(14,5,112):** 01234506173850912340561a2073b124053812c063192704135780a1273d069581c63052469850c73695b814ac98523c4795086391428596

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**(16,5,285):** 94f7cd02e8a3c605b72d80569b713cf59e40b619ef240ac58e27d94fa278bd935e17b062d83b01462ce7a049fb61c49adfb57039d284fa5d23684e09c26b1d83e6bcf1d7925bf4a61c7f458a602be48d3fa508de13f9b47d16c83e9167ac824d06af51c72af0351bd69f38ea50b389cea46f28c173e94c12573df8b15a0c72d5abe0c6814ac3950b6e34795f1ad48

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**(11,6,25):** 01234567018395a7123456701

**(12,6,33):** 01234567018926a317b96435709812347

**(13,6,47):** 012345607183940a1b35290cb6579140ba7831052a76190

**(14,6,66):** 012345607183940a12354b061c9723068db725610978a564b972305698170ca629

**(15,6,89):** 012345607182930a142b35061743c085d1230469157038a1e743bad06738bcd2a961cb475869ac037892abdc8

**(16,6,117):** 012345607182930a142b35061743c085d1230469157038a1420e361f25073b124086915e0342cbdea50319845b3d9607132489e012cd9ab4e0235

**(17,6,200):** 458g73bc40g8ef190d45ea9178b2a6ef732b014c3g780dc4abe5d901a65e347f62ab3gf7de08gc34d98067a195de621ag03b2f67gcb39ad4c8g0954d236e519a2fe6cdg7fb23c87g569084cd5109fg2a1e56fba289c3b7fg843c125d40891ed5bcf6ea9b

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**(14,7,42):** 0123456708914a6b03c94567d32a9417803ab46578

**(15,7,55):** 0123456708194a2b031c4562081dce597821bc39a4865b7901283ba

**(16,7,72):** 0123456708192a3b041c253d06172e3f094a217c59ba813cd49021bc56749adbce35421

**(17,7,98):** 041c253d06172e48031f259406172a3b051g789dc0b324ed109ab76de2c0153be89a0124cefd3b072e95dg0123456c081g