

A complete resolution of the Keller maximum clique problem *

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Abstract

A d -dimensional Keller graph has vertices which are numbered with each of the 4^d possible d -digit numbers (d -tuples) which have each digit equal to 0, 1, 2, or 3. Two vertices are adjacent if their labels differ in at least two positions, and in at least one position the difference in the labels is two modulo four. Keller graphs are in the benchmark set of clique problems from the DIMACS clique challenge, and they appear to be especially difficult for clique algorithms. The dimension seven case was the last remaining Keller graph for which the maximum clique order was not known. It has been claimed in order to resolve this last case it might take a “high speed computer the size of a major galaxy”. This paper describes the computation we used to determine that the maximum clique order for dimension seven is 124.

1 Keller Graphs

A d -dimensional Keller graph, G_d , has 4^d vertices which are numbered with each of the 4^d possible d -digit numbers which have each digit equal to 0, 1, 2, or 3. Two vertices are adjacent if their labels differ in at least two positions, and in at least one position the difference in the labels is two modulo four. The goal of our research was to find the maximum clique order in the graph G_7 , the only case that had not previously been solved.

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Corrádi and Szabó [7] determined that the Keller graphs of dimensions 1-5 have maximum cliques of orders 1, 2, 5, 12, and 28 respectively. For dimension six, the published results indicate that the maximum clique order is at least 60 and at most 64. However, David Applegate working in conjunction with Peter Shor ran a computation determining that the maximum clique order is 60. It had previously been determined that the maximum clique order for G_7 is at least 124 but at most 128, but now we know that the answer is 124.

These graphs have an interesting history, arising from a mathematical conjecture. They have also been frequently used as benchmarks for testing clique algorithms. The mathematical story is given in Section 2 and the computational background is in Section 3. The rest of the paper describes our new contributions.

2 Mathematical History

This section provides a historical survey of Minkowski’s and Keller’s cube-tiling conjectures. One place to find a more detailed history is the first chapter of this book[23], which is an expansion of Stein’s survey article in the *American Mathematical Monthly* [24]. One can view it as a case study of one interesting thread of mathematical research, winding over a hundred years (through three centuries) and among several diverse areas of mathematics.

What are these conjectures? Minkowski’s conjecture is

CONJECTURE 2.1. (MINKOWSKI) *Every lattice tiling of \mathbb{R}^n by unit cubes contains two cubes that meet in an $n - 1$ dimensional face.*

Keller’s conjecture is nearly the same; we merely drop the word *lattice*:

CONJECTURE 2.2. (KELLER) *Every tiling of \mathbb{R}^n by unit cubes contains two cubes that meet in an $n - 1$ dimensional face.*

A tiling of \mathbb{R}^n by unit cubes is a set of unit cubes such that every point in \mathbb{R}^n is covered by one of the

cubes, and such that the interiors of no two cubes overlap. We can assume that all the cubes are aligned parallel to the coordinate axis, although the conjectures are equivalent with or without this assumption. Two cubes thus meet in an $n - 1$ dimensional face if their centers differ by exactly one in one coordinate, and are equal in the other $n - 1$ coordinates.

Minkowski's conjecture arose originally in 1896 while Minkowski was considering a problem in Diophantine approximation. Investigating when an inequality was tight led Minkowski to formulate his conjecture, a problem in high-dimensional geometry. He originally stated it as a theorem, the proof of which he promised to publish at a later date. Eleven years later, he stated it as an open problem, leading one to suspect that he discovered a hole in an earlier proof. In 1938, in his Ph.D. thesis, Hajós turned Minkowski's conjecture into a problem in the theory of abelian groups. Three years later, he solved it using algebraic methods (the proof can be found in [23]).

Meanwhile, in 1930, Keller generalized Minkowski's cube-tiling conjecture to what has come to be known as Keller's cube-tiling conjecture. In 1940, Oskar Perron published a paper proving Keller's conjecture in six and fewer dimensions [19]. (He simultaneously published a paper proving Minkowski's conjecture in eight and fewer dimensions.) Even though the original motivation for Keller's conjecture disappeared with Hajós' 1941 proof of Minkowski's conjecture, it still appealed to some mathematicians as an intrinsically interesting question. Corrádi and Szabó [7], in the late 1980's, turned Keller's conjecture into a combinatorial problem, and attempted to find a counterexample via computer search. They showed that Keller's conjecture is true if and only if the Keller graph G_d has no cliques of order 2^d for all d .

Jeff Lagarias heard about the Keller conjecture early in 1991 from Victor Klee, who gave a lecture on interesting geometry problems at a meeting in Oberwolfach, Germany. Jeff told Peter Shor about it and in 1992, they found a counterexample in 12 dimensions which they were promptly able to reduce to ten dimensions [13]. In 2000, John Mackey [14] found an eight-dimensional counterexample, leaving the conjecture open only for seven dimensions. The computation described in this paper proves that the Keller graph G_7 has no clique of order 128, which implies that there is no counterexample to Keller's conjecture in seven dimensions with cubes whose coordinates are integers or half-integers. This is very strong evidence that Keller's conjecture is true in seven dimensions, as all the other counterexamples that have been found have been tilings with integer and half-integer coordinates.

3 Computational Experiments with Keller Graphs

Because the clique problem is NP-complete, it is unlikely that someone can find a polynomial time algorithm for its solution. This impedes searches for a computer aided resolution of the problem. Corrádi and Szabó [7] nevertheless did a computer search for counterexamples, and were able to show by computer that there were no counterexamples in dimensions less than or equal to five. Note that this is one fewer dimension than Perron was able to resolve by hand nearly fifty years earlier.

DIMACS hosted a challenge for Cliques, Colouring and Satisfiability in 1993 [12]. The repository for the challenge included a simple clique algorithm written by David Johnson, and a collection of benchmark clique problems. To illustrate how hard this clique-finding problem is, Peter Shor added these Keller graphs to the challenge repository. While most of the entrants found the right answer in dimension 5, only two of the entrants found the right answer in dimension 6, and nobody was able to get close to the largest clique that had been determined so far for dimension 7 (124 vertices). Later, David Applegate wrote a program that used some of the structure of this graph to perform an exhaustive search for counterexamples. While the program managed to show that there was no 64-clique in G_6 , it spent several days trying to attack the case of dimension 7 and made no discernible progress.

Marconi and Foster state that several properties of the Keller graphs make them especially difficult for genetic algorithms [16]. It has been conjectured that it could take a "high speed computer the size of a galaxy" to resolve the last open case (dimension 7) for the Keller clique problem [6, p. 24]. However, the techniques applied here accomplished this task using computation which only takes about 40 days on one machine (Section 7). Furthermore, the maximum clique order was determined to be 124 (Section 9, the Keller clique problem only asks whether the maximum clique order is 128 or less than 128).

Because the Keller graphs are vertex transitive, finding a k -clique in a Keller graph is equivalent to finding a $k - 1$ -clique in the graph H_d which is the subgraph of G_d induced by the neighbours of one of the vertices. Most clique algorithms for Keller graphs are run with H_d instead of G_d and it was actually H_4 , H_5 , H_6 , and H_7 that were added to the clique challenge repository (they have 171, 776, 3351, and 14190 vertices). Since then, there has been a large number of heuristics for the maximum clique problem that have been tested on these graphs.

In order to unify the results, they are expressed

here in terms of the clique order which is implied in the original graph G_d . The maximum clique orders for G_4 , G_5 , G_6 and G_7 are 12, 28, 60 and 124 respectively.

Some heuristics fail on dimension four with a maximum clique found of order 8 [21], 10 [5, 1], or 11 [8] instead of 12. In [3], the clique orders found with its four heuristics ranged from 8 to 11 for dimension 4. Others fail on dimension five. Some of these used several trials or more than one heuristic and their results were (18, 21, 24) [11], (23, 22, 23) [18], and (24, 27, 27) [4] instead of 28. The ones which fail on dimension 6 fell short of 60 with 54 [15], 55 [9], and (56,57) [25]. These two heuristics [22, 20] were able to find cliques of order 60 for dimension 6. Homer and Peinado [10] succeeded for dimension six but only found 120 instead of 124 for dimension seven.

4 Colouring Keller Graphs

A legal *vertex colouring* of a graph assigns a colour to each vertex so that adjacent vertices are different colours. A specific colouring of the Keller graph vertices is exploited by the clique algorithm. Understanding this colouring is critical for verification of the isomorphism screening described in Section 6.

THEOREM 4.1. *The Keller graph G_d can be coloured using 2^d colours.*

Proof. The vertices of G_d can be placed into a 2^d by 2^d array so that each row is an independent set (and each column is an independent set, but this information is not used for our solution). The numbering for the rows and columns is from 0 to $2^d - 1$. To compute the binary representation of the row number for a vertex, replace each 0/1 digit with 0 and each 2/3 digit with 1. To compute the binary representation of the column number, replace each 0/3 digit with 0 and each 1/2 digit with 1. For example, the array for dimension 3 is:

000	001	010	011	100	101	110	111
003	002	013	012	103	102	113	112
030	031	020	021	130	131	120	121
033	032	023	022	133	132	123	122
300	301	310	311	200	201	210	211
303	302	313	312	203	202	213	212
330	331	320	321	230	231	220	221
333	332	323	322	233	232	223	222

The tuples in the same row form an independent set because in each digit, the value is always either 0/1 or it is 2/3. Therefore there is no position where the difference is two modulo four.

COROLLARY 4.1. *A Keller graph of dimension d has maximum clique order at most 2^d .*

Proof. By Theorem 4.1, the Keller graph of dimension d is 2^d -colourable, and any clique contains at most one entry from each colour class.

The next theorem implies that if there is a counterexample for dimension d which corresponds to a 2^d -clique in G_d , then this can be used to construct a counterexample for all dimensions greater than or equal to d . Our proof is combinatorial whereas the proof by Corrádi and Szabó [7] is group theoretic.

THEOREM 4.2. *If a Keller graph of dimension d has a clique of order r then the Keller graph of dimension $d+1$ has a clique of order $2r$.*

Proof. Make a copy of the tuples in the clique of order r and then prefix each tuple with the digit 0 and call this collection of r $(d+1)$ -digit tuples A. Make a second copy of the tuples in the clique of order r . For each of the tuples, add 1 to each of the digits where this addition is done modulo 4. Then prefix each tuple with the digit 2. Call this second collection of r $(d+1)$ -tuples B.

We now prove that $A \cup B$ is a clique of order $2r$ in the $(d+1)$ dimension graph. Within the tuples in A, each pair of tuples differs in at least two positions and differs by two in one position because the tuples used to build A induce a clique in the dimension d graph. The same is true for B because adding one to each entry means that if a pair of tuples differ in at least two positions and differ by two in one position, they still do.

The tuples in A and the tuples in B differ by two in the first position since the first digit of those in A is 0 and the first digit for those in B is 2. So it remains to prove that each pair of tuples (a, b) with a selected from A and b selected from B differ in at least two positions. Suppose that they do not. This means that there exists one tuple in A which is $0t$ and one in B which is $2t$ for some d -dimensional tuple t . But then t was in the original clique and so was the tuple u created by subtracting one from each digit of t where the subtraction is done modulo four. But then u and t are tuples in the original clique which differ by one in every position which means they are not adjacent. This is a contradiction since the tuples from the original clique must be pairwise adjacent to each other.

5 Finding Maximum Cliques in a Keller Graph

The clique algorithm used is a variant of the clique algorithm proposed by Balas and Yu [2]. A simpler variant is used in [17]. The key idea is that any clique of the graph contains at most one vertex per colour class. The algorithm backs up when encountering any subproblems with the number of colour classes remaining less than the number of clique vertices required.

Bit twiddling was crucial in order to get the algorithm running fast enough to be practical. The graph and the sets of vertices which are candidates for a maximum clique are stored in a compressed format in 32-bit integers. When adding a new clique vertex, the algorithm always selects a colour class with a minimum number of options. Vertices in a colour class are stored in contiguous positions which facilitates quick counting of the number of choices remaining for each colour class. The graphs searched are selected as described in Sections 7, 8, and 9 so that in the clique problems solved, exactly one vertex must be chosen from each colour class. That is, if the algorithm reaches a state where a colour class includes no options for addition to the current clique, the algorithm can back up.

6 Automorphisms of the Keller Graphs

This section explains some symmetries of the graph that can be taken into account to shorten the search. Some operations that provide an automorphism of the Keller graph are:

1. Choose a tuple t and add t to each vertex label (modulo 4).
2. Choose a permutation and apply it to the d columns of every d -tuple.
3. Choose one position and interchange 0's and 2's in this position in all the tuples.
4. Choose one position and interchange 1's and 3's in this position in all the tuples.
5. Choose one position, and in this position the symbols 0, 1, 2, 3 are renumbered as 1, 0, 3, 2.

These operations are automorphisms because they preserve the number of positions that each pair of tuples agrees in and they also preserve the number of positions in which a pair of tuples has a difference of two. Thus it is obvious that they preserve adjacency. A *colouring preserving automorphism* is one such that if you consider each subset of vertices in a colour class corresponding to one row as defined by Theorem 4.1, these all end up the same colour after the automorphism is applied (that is, they all map to the vertices in the same row). Operations 2, 3, 4, and 5 above are colouring preserving. Operation 1 is colouring preserving if all the digits of t are equal when considered modulo two.

THEOREM 6.1. *Consider the ordering of the vertices of the Keller graph as indicated in Theorem 4.1 and the colour classes which are provided by the rows for this labelling. Then given any two colour classes r and c ,*

there is a colouring preserving automorphism that maps r to c .

Proof. Consider the i th digit, for $i= 0, 1, 2, \dots, (d-1)$ of the tuples in a colour class. Because of the way the colour classes are constructed, within one colour class, each digit position contains digits which are always either 0/1 or they are always 2/3. Create a vector v as follows: for each i , if colour class r and c both have 0/1 or both have 2/3 as the values in position i then v has 0 in position i . If one has 0/1 and the other has 2/3 then v has 2 in position i .

Note that colour class r has two choices for the digit in each position and since it has size 2^d , this means that colour class r actually has all such possible tuples. Therefore, adding the constructed vector v to each tuple from the graph is a colouring preserving mapping which maps the vertices of colour r to those of colour c .

THEOREM 6.2. *If the Keller graph G_d of dimension d has a clique of order $2^d - 1$ then there is a clique of order $2^d - 1$ in the graph H obtained by removing all the vertices in the last colour class.*

Proof. Consider a clique of the original graph G_d of order $2^d - 1$ that contains a vertex u from the last colour class. There is exactly one row and exactly one column of the original Keller graph which does not contain a vertex from this clique. Take the tuple t which is the entry in this missing row and missing column. Choose a colour preserving automorphism as per the proof of Theorem 6.1 which maps t to a vertex in the last colour class. This maps the clique to one which has the last colour class missing.

7 Case 127 or less than 127

In order to solve the last remaining case (dimension seven) for the Keller clique problem, it is only necessary to determine if the maximum clique order is 128 or less than 128. Thus, a conclusion that the maximum clique order is less than 127 suffices. The computation used for this took 15 hours running on 64 CPU's (about 40 days if run on only one machine). This is far less than the estimated time predicted for such a search. This section describes the theory for this case in detail.

As observed in the previous section, a colour class represented by a row has all of the tuples which have each position of the tuple taking on either 0/1 or 2/3. A colour class is represented by the lexicographically smallest tuple of a vertex in its class.

Using this notation, Theorem 6.2 of the previous section says that if the dimension seven Keller graph has a clique of order 127, then the graph H created by removing the vertices in the colour class 2222222 has

a clique of order 127. A search on this graph can be expedited by taking further graph automorphisms into consideration as indicated in the next theorem.

THEOREM 7.1. *Let H be the graph obtained from a dimension seven Keller graph by removing the colour class 2222222. Then there is an automorphism mapping any clique of order 127 in H to one which contains one of 95 3-cliques from the first three colour classes: 0000000, 0000002, and 0000020.*

Proof. Applicable automorphisms from the original Keller graph are colour preserving automorphisms that map the first three colour classes to each other, and the last colour class (the one removed) to itself. One applicable operation is to choose any one column and interchange 0/1 and also interchange 2/3 (Operation 5 of Section 6). Because this is permitted, the tuple chosen from the first row can be manipulated so that it is all 0's.

The first five columns of the first three tuples (selected respectively from the colour classes 0000000, 0000002, and 0000020) must then contain $(0, 0, 0)^T$, $(0, 0, 1)^T$, $(0, 1, 0)^T$ or $(0, 1, 1)^T$. Because we can permute these first 5 columns, we can assume that the seven columns in the first three tuples are in sorted order like this:

0	0	0	0	0	0	
0	0	1	1	w	x	
0	1	0	1	y	z	
-	-	-	-	-	-	
a	b	c	d	1	1	

where a , b , c , and d are the number of occurrences of each of the first four types of columns, $a + b + c + d = 5$.

Because the three vertices are in a clique, it is necessary that $x = 2$ and $y = 2$.

The analysis is broken into four cases depending on the values of w and z . Enumerating the potential values for a, b, c , and d in these four subcases and eliminating isomorphic situations results in 95 possibilities.

The search for determining if the answer is 127 or less than 127 used the graph H from Theorem 7.1. The clique algorithm considered each of the 95 ways to choose the clique vertices from the first three colour classes. The conclusion was that the Keller graph of dimension seven has no clique of order 127.

8 Case 126 or less than 126

For the case 126 or less than 126 a similar approach is applied. But there are now seven ways up to isomorphism to remove two colour classes.

THEOREM 8.1. *There are seven ways up to isomorphism to choose two colour classes to delete from the*

graph. These cases are equivalent to the ones you get from deleting the colour class 0000000 and one of these:

Case 1:	0	0	0	0	0	0	2
Case 2:	0	0	0	0	0	2	2
Case 3:	0	0	0	0	2	2	2
Case 4:	0	0	0	2	2	2	2
Case 5:	0	0	2	2	2	2	2
Case 6:	0	2	2	2	2	2	2
Case 7:	2	2	2	2	2	2	2

Proof. A combination of operations 3, 4, and 5 from Section 6 can be used to renumber so that 0000000 is one of the colour classes deleted. Permuting columns is an operation which is a colour-class preserving automorphism. So the second class can be normalized to be s 0's followed by $(7 - s)$ 2's.

These classes were replaced with equivalent ones which avoid the first three colour classes. The numbers of ways to select the 3-cliques up to isomorphism from the first three colour classes are: 145, 95, 251, 251, 95, 251, and 95 respectively. These numbers were checked by hand and using a computer program. It took about one week on 64 machines to run all 1183 cases. We discovered that the Keller graph of dimension seven has no cliques of order 126.

9 Case 125 or less than 125

This section describes the computation for the last and hardest case (determining that the Keller graph of dimension seven has no clique of order 125). The number of ways to remove three colour classes in all ways up to isomorphism is 23. The representatives for these cases were chosen so that the colour classes 0000000, 0000002, and 0000020 are not deleted so that in the next step, the first three clique vertices can be selected from these in all ways up to isomorphism.

The number of ways to select three clique vertices from the first three colour classes is different for each of these 23 cases. The symmetries applied must map the deleted classes to deleted classes and the first three classes to each other. The number of ways to select the first three clique vertices are: 95 (1 case), 145 (4 cases), 251 (5 cases), 365 (3 cases), 381 (2 cases), 553 (6 cases), and 747 (2 cases). These 8599 subproblems were solved with the conclusion that the Keller graph of dimension seven has no clique of order 125.

It is critical to double check proofs that are done on the computer. The algorithm was programmed independently by two different programmers. Both versions were run on smaller Keller graphs and it was confirmed that the number of recursive calls at each level matched.

The search for a 125-clique was done twice. One

program was run on a distributed system with 64 CPU's. The distribution was accomplished by having all jobs do a complete computation down to level 12 (the level corresponds to the number of clique vertices placed). Each machine was assigned an integer *slice number* ranging between 0 and 63. The computation was continued at level 12 whenever the number of visits to level 12 was congruent to the slice number modulo 64. The computation took 109 days in this environment. This means of dividing the work resulted in a very even split. All machines finished on the same day (after 109 days of computation!) with the longest job (measured by the last update times for the output files) taking just 17 hours longer than the shortest one.

Code was added to the other program so it could be run on the Kraken computer, a system which allows parallel computation and has 8192 CPU's. The computation was much faster with the additional CPU's and it took only a few weeks to finish.

When it had been confirmed that no 125-clique exists, a search was made to ensure that the program could find 124-cliques. The program found some but we did not do a complete search (this would require further isomorphism screening and would take longer than the search for 125).

10 Conclusions and Future Research

The maximum clique order for dimension seven is 124. One open question is determining all solutions of order 124 up to isomorphism. It is easy to see that there is more than one solution up to isomorphism by examining the number of times each symbol appeared in two of the solutions that we discovered. One of the maximum cliques came from doubling a solution of dimension six as per Theorem 4.2 then adding four more vertices (each of 0 and 2 appears 60 times in one position). In the other one, the maximum number of times a symbol appears in one position is 40.

Our result proves that there is no counterexample to Keller's conjecture in seven dimensions with cubes whose coordinates are integers or half-integers. The dimension seven case is still open however if arbitrary coordinates are used.

Because the Keller graphs have been used so often as benchmarks, we know that these are especially difficult graphs for heuristics that have been proposed. Can heuristics be found with better performance on Keller graphs? Which other classes of graphs are especially difficult for clique algorithms?

The structure exploited in solving this clique problem arises often in design theory problems. Which open questions in design theory can be resolved with a similar approach?

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