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A Kochen-Specker System Has at Least 22 Vectors

Sander UIJLEN and Bas WESTERBAAN

Radboud Universiteit, M1.05.11B P.O.Box 9010 6500 GL Nijmegen,
THE NETHERLANDS

{suijlen,bwesterb}@cs.ru.nl

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Abstract At the heart of the Conway-Kochen Free Will Theorem and Kochen and Specker's argument against non-contextual hidden variable theories is the existence of a Kochen-Specker (KS) system: a set of points on the sphere that has no $\{0,1\}$ -coloring such that at most one of two orthogonal points are colored 1 and of three pairwise orthogonal points exactly one is colored 1. In public lectures, Conway encouraged the search for small KS systems. At the time of writing, the smallest known KS system has 31 vectors.

Arends, Ouaknine and Wampler have shown that a KS system has at least 18 vectors, by reducing the problem to the existence of graphs with a topological embeddability and non-colorability property. The bottleneck in their search proved to be the sheer number of graphs on more than 17 vertices and deciding embeddability.

Continuing their effort, we prove a restriction on the class of graphs we need to consider and develop a more practical decision procedure for embeddability to improve the lower bound to 22.

§1 Introduction

1.1 The Experiment

Consider the following experiment. Shoot a deuterium atom (or another neutral spin 1 particle) through a certain fixed inhomogeneous magnetic field, such as that in the Stern-Gerlach experiment. The particle will then move undisturbed or deviate. What we have done is measure the spin component^{*1} of the particle along a certain direction. This direction depends on the specifics of the field and the movement of the particle.

 $^{^{*1}}$ As we are only interested in whether the particle deviates or not, we actually only consider the square of the spin component.

Quantum mechanics only predicts the probability, given the direction, whether the particle will deviate. Its probabilistic prediction has been thoroughly tested. One wonders: is there a *deterministic* theory predicting the outcome of this experiment?

Kochen and Specker have shown that such a non-contextual deterministic theory must be odd: it cannot satisfy the plausible SPIN axiom, that is:

SPIN Axiom (see 5)

Given three pairwise orthogonal directions. In exactly one of the directions, the particle will not deviate.

Their argument is based on the existence of a Kochen-Specker system.

Definition 1.1

A Kochen-Specker (KS) system is a finite set of points on the sphere^{*2} for which each pair is not antipodal and there is no **010-coloring**. A 010-coloring is a $\{0,1\}$ -coloring of the points such that^{*3}

- 1. no pair of orthogonal points are both colored 1 and
- 2. of three pairwise orthogonal points exactly one is colored 1; or alternatively: they are colored 0, 1 and 0 in some order.

A point on the sphere obviously corresponds to a direction in space. Because of this, the terms point, vector and direction can be used interchangeably. Antipodal points correspond to opposite vectors and these span the same direction in space.

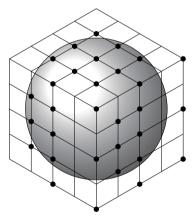


Fig. 1 John Conway's 31 Vector Kochen-Specker System

^{*2} We define KS systems to be three dimensional, as in the original proof of Kochen and Specker. Later, higher dimensional systems have been studied. See, for instance ^{12, p. 201}).

^{*3} In other papers, like ²⁾, the 0 and 1 are swapped; they consider 101-colorings. These colorings are of course equivalent and the difference arises from considering either squared spin measurements S_v^2 , or $1 - S_v^2$ for spin in direction v.

Suppose there is a KS system and a non-contextual deterministic theory satisfying the SPIN Axiom. Then we color a point of this system 0, whenever this theory predicts that the particle will deviate if the spin is measured in the direction corresponding to that point, and 1 otherwise. Given two orthogonal points of the system, we can find a third point orthogonal to both of them. The SPIN axiom implies exactly one of them is colored 1, so they cannot both be colored 1. Similarly, given three pairwise orthogonal vectors in the system, the SPIN axiom implies exactly one of them is colored 1. Hence there would be a 010-coloring of the KS system, quod non. Therefore a deterministic non-contextual theory cannot satisfy the SPIN Axiom.

The KS system proposed by Kochen and Specker contained 117 points.⁷⁾ Penrose and Peres¹¹⁾ independently found a smaller system of 33 points. The current record is the 31 point system of Conway.^{12, p. 197)} See Fig. 1. As pointed out by ^{2,3)}, finding small KS systems is of both theoretical and practical interest. In public lectures, Conway himself, stressed the search for small KS systems.⁹⁾

Before we continue, we would like to make two remarks.

- 1. There is an inconsistency in the literature on how to count the number of points in a Kochen-Specker system. One way is to take the minimal number of points required to be non-010-colorable. This is how we count in this paper. Another way is to require that for every pair of orthogonal points in the system, there is a third point orthogonal to both. This way of counting is for example used in ¹⁰⁾.
- 2. We consider three-dimensional Kochen-Specker systems for two reasons. First, every 3-dimensional system can be seen as a higher-dimensional system. The converse is false. Secondly, the size of the least Kochen-Specker system in dimension 4 and higher has already been found.¹⁰⁾ The three-dimensional case is still open.

1.2 Overview

In ²⁾ Arends, Ouaknine and Wampler (AOW) give a computer aided proof that a KS system must have at least 18 vectors. We improve their lower bound and show that a KS system must have at least 22 vectors.

First, in Subsection 1.3, we repeat a part of AOW's work, in particular the reduction of KS systems to graphs. The bottleneck of their search was the sheer number of graphs and the deciding whether such graphs are embeddable. In Section 2, we improve upon their reduction, to cut down the number of graphs to consider drastically, and state the results of our main computation. Finally, in Section 3, we describe our practical embeddability test. In Section 4, we discuss related work. The software and results of the various computations performed for this paper, can be found here.¹⁶⁾

This is an extended version of the paper published in proceedings of the 11th workshop on Quantum Physics and Logic.¹⁷⁾ Compared to the results presented on the workshop, we have improved the lower-bound to 22. We also include new restrictions on the graph enumeration of which we would like to

emphasize Prop. 2.2, which promises to push the bound when implemented efficiently. Furthermore we expand on methods to prove unembeddability. Finally we discuss how the related results in the literature compare to ours.

1.3 Kochen-Specker Graphs

We follow ²⁾ and reduce the search for Kochen-Specker systems to the search for a certain class of graphs. First note that in a Kochen-Specker system we may replace a point with its antipodal point. They are both orthogonal to the same points and hence the non-010-colorability is preserved. Therefore, we may assume antipodal points are identified on the sphere. That is: a Kochen-Specker system is a finite subset of the projective plane that is not 010-colorable.

Definition 1.2

Given a finite subset S of the projective plane (or equivalently, a finite subset of the northern hemisphere without equator**). Define its **orthogonality graph** G(S) as follows. The vertices are the points of S. Two vertices are joined by an edge, if their corresponding points are orthogonal.

Definition 1.3

A graph G is called **embeddable**, if it is a subgraph of an orthogonality graph. That is: if there is a finite subset S of the projective plane, such that $G \leq G(S)$.

Definition 1.4

A graph is called **010-colorable** if there is a $\{0,1\}$ -coloring of the vertices, with

- 1. for each triangle there is exactly one vertex that is colored 1 and
- 2. adjacent vertices are not both colored 1.

Definition 1.5

A Kochen-Specker graph is an embeddable graph that is not 010-colorable.

It is an easy, but important, consequence of the definitions that:

Fact 1.1

A finite subset S of the projective plane is a Kochen-Specker system, if and only if its orthogonality graph G(S) is Kochen-Specker.

To prove there is no Kochen-Specker system on 17 points, it would be sufficient to enumerate all graphs on 17 vertices and check these are not 010-colorable or not embeddable. However, this is infeasible as there are already $\sim 10^{26}$ non-isomorphic graphs on 17 points.¹³⁾ Luckily, we can restrict ourselves to certain classes of graphs.

Proposition 1.1 (by 2)

An embeddable graph is squarefree. That is: it does not contain the square \si

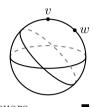
^{*4} A subset of the projective plane can be identified with a subset of the closed northern hemisphere. For a finite subset we can always rotate in such a way that no points lie on the equator.

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as a subgraph.*5

Proof

Given two non antipodal points $v \neq w$. See the figure on the right. Consider the points orthogonal to v. This is a great circle. The points orthogonal to w is a different great circle. They intersect in precisely two antipodal points. Hence, if c and d are points, both orthogonal to v and w, then c and d are equivalent. Therefore, an embeddable graph cannot contain a square.



The squarefreeness is a considerable restriction. There are only $\sim 10^{10}$ non-isomorphic squarefree graphs on 17 vertices.¹⁴⁾ Next, we show we can restrict ourselves to connected graphs.

Proposition 1.2 (by 2)

A minimal Kochen-Specker graph is connected.

Proof

Suppose G is a disconnected Kochen-Specker graph. Then one of its components is not 010-colorable. As a subgraph of an embeddable graph is embeddable, this component is embeddable as well. Hence it is a smaller connected Kochen-Specker graph.

The gain, however, is small. There are only $\sim 10^9$ non-isomorphic squarefree graphs on 17 vertices that are disconnected. In our computations, checking for connectedness required more time than would be gained by reducing the number of graphs. Cf. Corollary 2.1.

We have verified the main result of ²⁾:

Computation 1.1

There is only one non-010-colorable squarefree connected graph on less than 18 vertices. See Fig. 2. It is not embeddable, as the graph in Fig. 3 is an

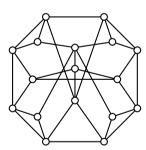


Fig. 2 AOW's 17-vertex Non-010-colorable Graph

^{*5} Some authors call a graph squarefree if it does not contain the square as induced subgraph. For them the complete graph on four vertices \(\mathbb{Z} \) is squarefree. We follow Weisstein \(\mathbb{18} \) and Sloane \(\mathbb{14} \) and call a graph squarefree if it does not contain the square as subgraph. For us the complete graph on four vertices is not squarefree.

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unembeddable subgraph. For our proof, see Proposition 3.1. Hence a Kochen-Specker system has at least 18 points.

§2 An Improved Lower Bound

Continuing the effort of Arends, Ouaknine and Wambler, we consider another restriction.

Proposition 2.1

A minimal Kochen-Specker graph has minimal vertex-order three. That is: every vertex is adjacent to at least three other vertices.

Proof

Given a minimal Kochen-Specker graph G. Suppose v is a vertex with order less than or equal to 2. Let G' be G with v removed. Clearly G' is embeddable. Suppose G' is 010-colorable. Then we can extend the coloring to a coloring of G as follows. If v is adjacent to only one or no vertex, then we can color v with 0. Suppose v is adjacent to two vertices, say v and v'. If one of v or v' is colored 1, we can color v with 0. If both v and v' are colored 0, we can color v with 1. This would imply v is 010-colorable, quod non. Therefore v is a smaller Kochen-Specker graph, which contradicts the minimality of v.

There are only $\sim 10^7$ squarefree non-isomorphic graphs on 17 vertices with minimal vertex order 3. Even though Arends, Ouaknine and Wampler note this restriction once, surprisingly, they did not restrict their graph enumeration to graphs with minimal vertex order 3. We present another considerable restriction.

Proposition 2.2

In a minimal Kochen-Specker graph, every vertex is part of a triangle.

Proof

Given any graph G together with a vertex v of G such that v is not part of a triangle. Let G' denote G without v. Suppose G' is 010-colorable. Then so is G, as we may extend the coloring of G' to G by coloring v with 0. Contraposing: if G is not 010-colorable, then G' is not 010-colorable. Clearly, if G is embeddable, then so is G'. Thus if G is Kochen-Specker, then so is G'.

There are only $\sim 10^5$ squarefree non-isomorphic graphs on 17 vertices with minimal vertex degree 3 where every vertex is part of a triangle. Unfortunately, we could not find an efficient algorithm to restrict the enumeration of graphs to those where every vertex is part of a triangle.

We continue with a strengthening of Proposition 1.2.

Proposition 2.3

A minimal Kochen-Specker graph is edge-biconnected. That is: removing any single edge leaves the graph connected.

We need some preparation, before we can prove this Proposition.

Definition 2.1

Given a graph G and a vertex v of G. We say, v has fixed color c (in G), if G is 010-colorable and for every 010-coloring of G, the vertex v is assigned color c.

We are interested in these graphs because of the following observation.

Lemma 2.1

If there is an embeddable graph G on n vertices with a vertex with fixed color 1, then there is a Kochen-Specker graph on 2n vertices.

Proof

Let G be a graph and v a vertex of G with fixed color 1. Consider two copies of the graph G. Connect the two instances of v with an edge. Call this graph G'. Clearly, G' is not 010-colorable.

We need to show G' is embeddable. Given an embedding S of G. We may assume that the point in S corresponding to v is the north pole. Furthermore, we may assume that there is no point on the x-axis, by rotating points along the north pole. Let S' be S rotated 90 degrees along the y-axis. Some points of S and S' might overlap. That is: there might be a point s in S and s' in S' that are equal or antipodal. Observe that if no points of S' and S' overlap, then $S \cup S'$ is an embedding of G'.

Suppose there are points in S' and S that overlap. Note that the north pole (and south pole) is not in S'. Let S'' be S' rotated along the north pole at some angle α . There are finitely many angles such that there are overlapping points. Thus there is an angle such that $S \cup S''$ is an embedding of G'.

Unfortunately, these graphs are not small.

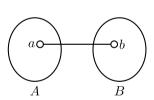
Computation 2.1

There are no embeddable graphs with fixed color 1 on less than 17 vertices.*6

We are ready to prove that a minimal KS graph is edge-biconnected.

Proof of Proposition 2.3

Given a minimal Kochen-Specker graph G. Recall it must be connected. Suppose it is not edge-biconnected. Then there must be an edge (a,b) in G, whose removal disconnects G. Thus G decomposes into two connected graphs A and B with $a \in A, b \in B$ and (a,b) is the only edge between A and B. Clearly A and B are embeddable.



Note that A must be 010-colorable, for if it were not 010-colorable, then A is a Kochen-Specker graph, in contradiction with G's minimality. Similarly B is 010-colorable. Suppose there is a 010-coloring of A in which a is colored 0. Then we can extend this coloring with any 010-coloring of B to a 010-coloring of G, which is absurd. Thus a must have fixed color 1 in A. Similarly b must have

^{*6} Source code at code/comp5.py of 16).

fixed color 1 in B. Thus by Computation 2.1, we have $\#A \ge 17$ and $\#B \ge 17$. Consequently $\#G \ge 34$. Contradiction with G's minimality.

We can go one step further.

Proposition 2.4

A minimal Kochen-Specker graph is edge-triconnected. That is: removing any two edges keeps the graph connected.

Again, we need some preparation. First, we generalize the notion of fixed color.

Definition 2.2

Given a graph G together with selected vertices $v_1, \ldots, v_n \in G$. The **type** t **of** (v_1, \ldots, v_n) (in G) is the set of all possible ways $\{v_1, \ldots, v_n\}$ can be 010-colored. That is:

$$t = \{(c(v_1), \dots, c(v_n)); c: G \to \{0, 1\}, c \text{ is a 010-coloring of } G\}$$

A type of n vertices is called an n-type.

Example 2.1

- The triangle & has 3-type $\{(1,0,0),(0,1,0),(0,0,1)\}.$
- Every vertex in a Kochen-Specker graph has type ∅.
- A vertex v has 1-type $\{(1)\}$ in G if and only if it has fixed color 1 in G.

Just as vertices with fixed color are rare, we are interested in types, because most types do not occur in small graphs.

Computation 2.2

We have enumerated all embeddable graphs of less than 17 vertices and determined a lower bound at which a particular 1- or 2-type occurs, omitting the trivial types $\{(0), (1)\}$ and $\{(0,0), (0,1), (1,0), (1,1)\}$.*

1/2-type	#G
$\{(0,0),(1,0),(0,1)\}$	non-trivially ≥ 10
$\{(0,0),(1,0),(1,1)\}$	≥ 10
$\{(0,0),(0,1),(1,1)\}$	≥ 10
$\{(0,0),(0,1)\}$	≥ 15
$\{(0,0),(1,0)\}$	≥ 15
$\{(0)\}$	≥ 15
$\{(0,1),(1,0)\}$	≥ 16
other	≥ 17

The type $\{(0,0),(1,0),(0,1)\}$ occurs in the embeddable two-vertex graph **O–O**. Because the two vertices are adjacent, this occurrence of the type is called trivial.

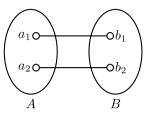
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^{*7} Source code at code/comp5.py of 16).

Proof of Proposition 2.4

Given a minimal Kochen-Specker graph G. Suppose it is not edge-triconnected. Then it splits

Suppose it is not edge-triconnected. Then it splits into two graphs A and B together with vertices $a_1, a_2 \in A$ and $b_1, b_2 \in B$ such that (a_1, b_1) and (a_2, b_2) are the only edges between A and B. Note that A and B must be 010-colorable, for otherwise G would not be a minimal Kochen-Specker graph.

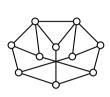


- 1. Suppose $a_1 = a_2$ and $b_1 = b_2$. Then G is not edge-biconnected. Contradiction with Proposition 2.3.
- 2. Suppose $a_1 \neq a_2$ and $b_1 = b_2$. Suppose $b_1 = b_2$ does not have a fixed color in B. Then any coloring of A can be extended with some coloring in B to a coloring of G. Contradiction. Apparently $b_1 = b_2$ has a fixed color in B.
 - a. Suppose $b_1 = b_2$ has fixed color 1 in B. Note $\#B \ge 17$ by Computation 2.2. Suppose there is a coloring of A in which both a_1 and a_2 have color 0. Then, regardless whether a_1 and a_2 are adjacent or not, this coloring can be extended with a coloring of B (in which $b_1 = b_2$ must be colored 1) to a coloring G. Contradiction. Thus the type of (a_1, a_2) in A cannot contain (0, 0). Thus, by Computation 2.2, $\#A \ge 17$. Consequently $\#G \ge 34$. Contradiction with minimality.
 - b. Apparently $b_1 = b_2$ has fixed color 0 in B. Hence, by Computation 2.2, $\#B \geq 15$. Suppose a_1 is not adjacent to a_2 . Then any coloring of A can be extended with a coloring of B to a coloring of G. Contradiction. Apparently a_1 is adjacent to a_2 . The type of (a_1, a_2) in A cannot contain (1, 0) or (0, 1) for otherwise G can be colored. It also cannot contain (1, 1) as a_1 and a_2 are adjacent. Thus both a_1 and a_2 have fixed color 0 in A. Hence $\#A \geq 17$ by Computation 2.2. Consequently $\#G \geq 32$. Contradiction with minimality.
- 3. Suppose $a_1 = a_2$ and $b_1 \neq b_2$. This leads to a contradiction in the same way as in case 2.
- 4. Apparently $a_1 \neq a_2$ and $b_1 \neq b_2$. The type of (a_1, a_2) in A cannot contain (0,0), for otherwise G is colorable. Similarly, the type of (b_1,b_2) in B cannot contain (0,0). Thus both $\#A \geq 17$ and $\#B \geq 17$. Hence $\#G \geq 34$. Contradiction with minimality.

Although these restrictions are theoretically pleasing, they seem to be of little use as a practical restriction. Concerning excluding disconnected graphs:

Computation 2.3

There are five non-isomorphic minimal squarefree connected graphs with minimal vertex order 3 and they have 10 vertices.*8 Three of them are embeddable and shown below. The remaining two are depicted in Computation 3.1.







Corollary 2.1

Any disconnected squarefree graph with minimal vertex order 3 has at least 20 vertices, for it has two connected components, each with at least 10 vertices. With 20 vertices, there are exactly 25 of these.

This justifies, at this stage, not checking for connectedness. Similarly, we believe there are very few connected but not edge-biconnected graphs.

Now we can state our main computation.

Computation 2.4

Let C_n denote the number of non-010 colorable squarefree graphs with minimal vertex order 3 on n nodes. Then:*9

All these 12339 graphs are not embeddable. See Computation 3.1.

The computation was distributed on approximately 300 CPU cores and took roughly three months. It was executed as follows. We enumerated all squarefree graphs with minimal vertex order 3 on less than or equal to 21 vertices,*¹⁰ using the geng util of the nauty software package, which uses the isomorphism-free exhaustive generation method of McKay.⁸⁾ The output of geng, we passed through a custom heuristic backtracker written in C++ to decide 010-colorability of these graphs.

§3 Embeddability

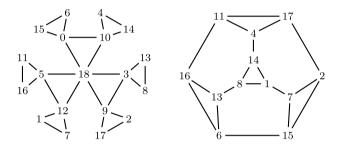
Our computation has yielded over nine-thousand non-010-colorable graphs. If we show one of them is embeddable, we have found a new KS system. If we demonstrate all of them are not embeddable, we have proven a lower bound on the size of a minimal KS system.

 $^{^{*8}}$ They are the first five graphs listed on: $\verb|http://kochen-specker.info/smallGraphs/|.$

^{*9} Source code at code/comp6 of 16).

 $^{^{\}ast 10}$ On 21 vertices, we found 24,888,945,914,244 such graphs.

In ²⁾, Arends, Wampler and Ouaknine discuss several computer-aided methods to test embeddability of a graph. None of these methods could decide for all graphs considered, whether they were embeddable or not. We propose a new method, which for all graphs we considered, could decide whether they were embeddable or not. But first, we give two pen-and-paper proofs of the non-embeddability of the following graph. These two pictures represent a single connected graph of minimal vertex degree three. For presentation, some vertices have been drawn twice.



3.1 First Pen-and-paper Proof

Of the graphs of 19 vertices, the above graph was the only not excluded by the unembeddable graphs known by AOW. In order to show that this graph is not embeddable, we proceeded as follows. If the graph is embeddable, there is always an embedding such that the coordinates on the sphere of some triangle in this graph are (1,0,0), (0,1,0) and (0,0,1). We chose to assign these values to the points 0, 10 and 18, respectively. For each of these vertices, any vertex adjacent to it must lie on a certain great circle. For example, we can assign to the vertices 9 and 3, which are both connected to 18, the coordinates $(\sqrt{1-x^2}, -x, 0)$ and $(x, \sqrt{1-x^2}, 0)$, for some $x \in (-1,1)$ and $x \neq 0$. We find similar expressions for the coordinates of the other triangles containing the vertices 0, 10 and 18. The remaining vertices are assigned a variable value on the sphere, where we always choose the component containing the square-root positive, so we obtain coordinates of the form $(a, b, \sqrt{1 - a^2 - b^2})$, for $a, b \in (-1, 0) \cup (0, 1)$. In this way we obtain no variables for the first triangle, 4 for attached triangles and then 16 for the left over vertices giving 20 unknowns. The relations for these variables are given by the fact that the inner product of the vectors should be zero if they are adjacent. Not counting the inner products that are trivially zero, we obtain 24 equations. By tedious calculations, one derives the equation $x^2(1-x^2)=-1$, which is not satisfiable. Hence this system is not embeddable.

If we only consider the points used to obtain the contradiction, we find an unembeddable subgraph of the system containing 13 vertices.*¹¹ In the appendix we included the derivation of contradiction. In theory, this approach can be

 $^{^{*11}}$ These are the vertices 0, 2, 3, 4, 6, 8, 9, 10, 13, 14, 15, 17 and 18.

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mechanically performed by a computer. However, there are too many variables to solve this in reasonable time.

3.2 Second Pen-and-paper Proof

We give a second simpler pen-and-paper proof of the unembeddability of the graph, by showing a subgraph is unembeddable.

Proposition 3.1

The graph in Fig. 3 is not embeddable.

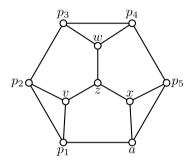


Fig. 3 One of The Two Minimal Non-embeddable Graphs

Proof

Suppose it is embeddable. Consider (the point associated to) p_1 . It is orthogonal to both a and v. Since a and v are not collinear, p_1 must be collinear to $v \times a$, the cross-product of v and a. Similarly, p_2 is collinear to $v \times p_1 = v \times (v \times a)$. Continuing in this fashion, walking the circumference of the graph, we find

a is collinear to
$$x \times (x \times (w \times (w \times (v \times (v \times a)))))$$
. (1)

Now, we may assume that z=(0,0,1) and x=(1,0,0). Thus: $v=(v_1,v_2,0)$; $w=(w_1,w_2,0)$ and $a=(0,a_2,a_3)$ for some $-1\leq v_1,v_2,w_1,w_2,a_2,a_3\leq 1$, with $v_1^2+v_2^2=1$; $w_1^2+w_2^2=1$ and $a_2^2+a_3^2=1$. Now, (1) becomes:

$$\begin{pmatrix} 0 \\ a_2 \\ a_3 \end{pmatrix} \text{ is collinear to } \begin{pmatrix} 0 \\ -a_2 v_1 w_2 (v_1 w_1 + v_2 w_2) \\ -a_3 (v_1^2 w_1^2 + v_1^2 w_2^2 + v_2^2 w_1^2 + v_2^2 w_2^2) \end{pmatrix}.$$

Consequently

$$v_1 w_2 (v_1 w_1 + v_2 w_2) = v_1^2 w_1^2 + v_1^2 w_2^2 + v_2^2 w_1^2 + v_2^2 w_2^2$$

$$= (v_1^2 + v_2^2) w_1^2 + (v_1^2 + v_2^2) w_2^2$$

$$= w_1^2 + w_2^2$$

$$= 1.$$

Since v and w are not collinear, we have by Cauchy-Schwarz $|\langle v, w \rangle| < 1$. Thus

$$1 > |v_1 w_2 \langle v, w \rangle| = |v_1 w_2 (v_1 w_1 + v_2 w_2)| = 1,$$

which is a contradiction. Apparently this graph is not embeddable.

3.3 An Algorithm to Decide Embeddability

In the previous proof, we fixed, without loss of generality, the position of a few vertices. Then we derived cross-product expressions for the remaining vertices. Finally, we found an equation relating some of the cross-product expressions and show it is unsatisfiable. We automate this reasoning as follows.

Algorithm 3.1

```
while there are unassigned vertices do
       pick an unassigned vertex v
       assign V(v) = v
       \max v as free
       while there are unassigned vertices adjacent to two distinct assigned do
5:
          pick such a vertex w adjacent to the assigned w_1 and w_2
          assign V(w) = V(w_1) \times V(w_2)
          mark edges (v, w_1) and (v, w_2) as accounted for
       end while
10: end while
   for each pair of vertices (v_1, v_2) do
       if (v_1, v_2) is not an edge then
          record requirement: "V(v_1) is not collinear to V(v_2)"
       end if
15: end for
   for each edge (v_1, v_2) not accounted for do
       record requirement: "V(v_1) is orthogonal to V(v_2)"
   end for
```

At two points in the algorithm, there is a choice which vertex to pick. Depending on the vertices chosen, the number of recorded requirements and free points may significantly vary. By considering all possible choices, one can find the one with least free points.

The requirements can be mechanically converted to a formal sentence in the language of the real numbers. This sentence is true if and only if the graph is embeddable. Famously, Tarski proved¹⁵ that such sentences are decidable. His decision procedure has an impractical complexity. However, its practical value has been improved by, for instance, the method of cylindrical algebraic decomposition.⁴ We have used the redlog⁶ package of the reduce algebra system, which implements a variant of Tarski's quantifier elimination.*¹²

Different assignments give different sentences. In our tests, some assignments would yield sentences that were decided within milliseconds, whereas another assignment with less free vertices would yield a sentence that could not be decided (directly). Therefore, when determining embeddability of a graph, we

^{*12} The reader can find the reduce script generated mechanically for the graph in Fig. 3 here: http://kochen-specker.info/smallGraphs/49743f49514769444f.html.

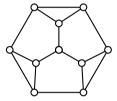
try several assignments in parallel.

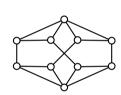
Using this algorithm, we could determine embeddability for most graphs with less than 15 vertices. However, there were a few (010-colorable) graphs for which the algorithm would not terminate and hence their embeddability was not decided. By hand, we found with trial and error an embedding for some of these graphs. Once we knew the troublesome graphs were embeddable, we adapted the algorithm, as to guess for some assignments the position of one of the vectors. If the corresponding sentence turns out false, we know nothing. However, if the sentence is true, we know the graph is embeddable.

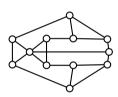
With this method, we have decided in a day the embeddability of every squarefree graph with minimal vertex order three of less than 15, except for one.*¹³ In particular:

Computation 3.1

Every squarefree graph of minimal vertex order three that is not 010-colorable of order less than or equal to 21 contains an unembeddable subgraph.*¹⁴ In particular, those of order less than or equal to 20 contains, as a subgraph, one of the following three graphs:







These three graphs are unembeddable. The left and middle graph are the only minimal unembeddable squarefree graph. For the first graph, we have proven directly that it is unembeddable. See Proposition 3.1. For the second graph, we also have a similar direct proof. See Proposition B.1 in the appendix. The third graph is shown not to be embeddable using our algorithm.

§4 Related Work

This paper improves the lower bound of Arends, Ouaknine and Wampler^{1,2)} on the size of a minimal Kochen-Specker system. Pavičić, Merlet, McKay and Norman¹⁰⁾ count the size of a Kochen-Specker system differently and have demonstrated a different bound.

^{*&}lt;sup>13</sup> A list of all squarefree graphs with minimal vertex order three of less than 15 vertices together with their embeddability can be found here: http://kochen-specker.info/smallGraphs/. The graph for which we could not determine embeddability can be found here: http://kochen-specker.info/smallGraphs/4d4b3f4b3f603f47414641654953625f3f.html.

^{*14} A list of these graphs together with their unembeddable subgraphs, can be found here: http://kochen-specker.info/candidates/. The source code for this computation can be found at code/comp2.py of ¹⁶).

Definition 4.1

A Kochen-Specker graph is called **complete** if every edge is part of a triangle.

Pavičić et al have given a lower bound on the size of the minimal *complete* Kochen-Specker system. Similar to our approach, they reduce the problem to a question about discrete structures which can be considered as a subclass of graphs. They discovered several uncolorable candidates of which they could prove unembeddability using either symbolic computation or interval analysis.

Clearly, a bound on the minimal size of a KS system is also a bound on the minimal size of a complete system. Conversely, a KS system can be completed by adding missing vectors. However, it is not clear how many vectors have to be added in general to complete the system. A history of the different bounds on 3-dimensional Kochen-Specker systems is given in the table below.

Authors	year	KS	complete KS
Kochen and Specker ⁷⁾	1975	≤ 117	≤ 192
Penrose, Peres ¹¹⁾ (independendly)	1991	≤ 33	≤ 57
Conway	~ 1995	≤ 31	≤ 51
$UW^{17)}$	2014	≥ 22	≥ 22
Pavičić et al. ¹⁰⁾	2004	?	≥ 30

Fig. 4 A history of the bounds on the size of the minimal (complete) three-dimensional Kochen-Specker system.

§5 Conclusion and Future Research

Arends, Ouaknine and Wampler struggled with two problems: enumerating candidate graphs of less than 31 vertices and testing their embeddability. We have verified most of their computations. Then we enumerated all candidate graphs up to and including 21 vertices. Furthermore, we have proposed a new decision procedure, which was able to decide embeddability for all candidate graphs we found. Therefore, we demonstrate: a Kochen-Specker system must have at least 22 points.*¹⁵

Enumerating all candidate graphs of less than 31 vertices is computationally infeasible. To bridge the enormous gap between 22 and 31, requires a new insight. Most likely, this would be a new practical restriction on which graphs to consider. In particular (following Prop. 2.2) a fast algorithm to enumerate square-free graphs of minimal vertex order three where each node is part of a triangle, would probably allow to test for KS-systems up to and including 24 vertices.

The reader, interested in pursuing this line of research, is encouraged to read the master thesis¹⁾ of Arends, in which he discusses in detail several other properties that a minimal KS system must enjoy, as well as some failed attempts.

 $^{^{\}ast 15}$ The authors have a wager whether there is a minimal KS system of less than 25 vertices.

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References

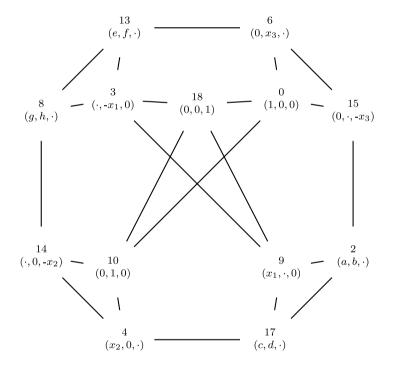
- Arends, F., "A lower bound on the size of the smallest kochen-specker vector system in three dimensions," Master's thesis, University of Oxford, 2009. http://www.cs.ox.ac.uk/people/joel.ouaknine/download/arends09.pdf.
- 2) Arends, F., Ouaknine, J. and Wampler, C. W., "On searching for small kochenspecker vector systems," in *Proc of the 37th international conference on Graph-Theoretic Concepts in Computer Science*, pp. 23–34, Springer-Verlag, 2011.
- 3) Cabello, A., "Kochen-specker theorem and experimental test on hidden variables," *International Journal of Modern Physics A*, 15, 18, pp. 2813–2820, 2000.
- 4) Collins, G. E., "Quantifier elimination for real closed fields by cylindrical algebraic decomposition," in *Quantifier elimination and cylindrical algebraic decomposition*, pp. 85–121 Springer, 1998.
- 5) Conway, J. H. and Kochen, S., "The strong free will theorem," *Notices of the AMS*, 56, 2, pp. 226–232, 2009.
- Dolzmann, A. and Sturm, T., "Redlog: Computer algebra meets computer logic," Acm Sigsam Bulletin, 31, 2, pp. 2–9, 1997.
- 7) Kochen, S. and Specker, E. P., "The problem of hidden variables in quantum mechanics," in *The Logico-Algebraic Approach to Quantum Mechanics*, pp. 293–328, Springer, 1975.
- 8) McKay, B. D., "Isomorph-free exhaustive generation," *Journal of Algorithms*, 26, 2, pp. 306–324, 1998.
- 9) Ouaknine, J., personal communication. Attended such a lecture of Conway at the Oxford Mathematical Institute in 2005.
- Pavičić, M., Merlet, J-P., McKay, B. and Megill, N. D., "Kochen-specker vectors," Journal of Physics A: Mathematical and General, 38, 7, pp. 1577–1592, 2005.
- Peres, A., "Two simple proofs of the kochen-specker theorem," Journal of Physics A: Mathematical and General, 24, 4, L175, 1991.
- 12) Peres, A., Quantum theory: concepts and methods, Springer, 1995.
- 13) Sloane, N. J. A., The On-Line Encyclopedia of Integer Sequences, http://oeis.org/A000088 (Number of graphs on n unlabeled nodes.).
- 14) Sloane, N. J. A., The On-Line Encyclopedia of Integer Sequences, http://oeis.org/A006786 (Squarefree graphs on n vertices.).

^{*16} http://jd7h.com/

- 15) Tarski, A., "A decision method for elementary algebra and geometry," RAND report R-109, RAND Corp., Santa Monica, CA.
- 16) Uijlen, S. and Westerbaan, B., Code and data for "a kochen-specker system has at least 22 vectors," https://github.com/bwesterb/ks.
- 17) Uijlen, S. and Westerbaan, B., "A kochen-specker system has at least 22 vectors (extended abstract)," in *Proc. of the 11th workshop on Quantum Physics and Logic, 172*, pp. 154–164, 2014.
- 18) Weisstein, E. W., Square-free graph, http://mathworld.wolfram.com/Square-FreeGraph.html (Last visited on may 6th 2014.).

Appendix A: Original Pen-and-paper Proof

In this appendix, we show by hand, that indeed the 19 vertex graph considered at the start of section 3 is not embeddable. We restrict the calculation to the 13-vertex unembeddable subgraph.



This is the subgraph and we have given the vertices names corresponding to the original, 19 vertex, graph. Below each name is a coordinate on the sphere (whenever there is a \cdot in the coordinate, we mean that this component of the coordinate is fixed by the other components, as it must be a point on the sphere, where we take this \cdot to be the positive square root).

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Now if two vertices are connected via an edge, we have that the inner product of their coordinates is zero. Vertices connected to the points 0,10 and 18 are trivially zero. The non trivial equations then become:

$$ax_1 + b\sqrt{1 - x_1^2} = 0 (2)$$

$$cx_1 + d\sqrt{1 - x_1^2} = 0 (3)$$

$$e\sqrt{1-x_1^2} - fx_1 = 0 (4)$$

$$g\sqrt{1-x_1^2} - hx_1 = 0 ag{5}$$

$$g\sqrt{1-x_2^2} - x_2\sqrt{1-g^2 - h^2} = 0 (6)$$

$$cx_2 + \sqrt{1 - x_2^2} \sqrt{1 - c^2 - d^2} = 0 (7)$$

$$b\sqrt{1-x_3^2} - x_3\sqrt{1-a^2-b^2} = 0 (8)$$

$$fx_3 + \sqrt{1 - e^2 - f^2}\sqrt{1 - x_3^2} = 0 ag{9}$$

$$ac + bd + \sqrt{1 - a^2 - b^2}\sqrt{1 - c^2 - d^2} = 0$$
 (10)

$$eg + fh + \sqrt{1 - e^2 - f^2}\sqrt{1 - g^2 - h^2} = 0$$
 (11)

From the equations containing only x_1 we can eliminate four variables.

$$b = \frac{-ax_1}{\sqrt{1 - x_1^2}} \tag{1'}$$

$$d = \frac{-cx_1}{\sqrt{1 - x_1^2}} \tag{2'}$$

$$e = \frac{fx_1}{\sqrt{1 - x_1^2}}\tag{3'}$$

$$g = \frac{hx_1}{\sqrt{1 - x_1^2}} \tag{4'}$$

Note that this is possible since all $x_i \in (-1,1)\setminus\{0\}$ since otherwise we would have coinciding coordinates of vertices in the graph.

Substituting these expressions in the other six equations and using that $\frac{x}{1-x}+1=\frac{1}{1-x},$ we obtain:

$$\frac{hx_1}{\sqrt{1-x_1^2}}\sqrt{1-x_2^2} - x_2\sqrt{1-\frac{h^2}{1-x_1^2}} = 0$$
 (5')

$$cx_2 + \sqrt{1 - x_2^2} \sqrt{1 - \frac{c^2}{1 - x_1^2}} = 0 ag{6'}$$

$$\frac{-ax_1}{\sqrt{1-x_1^2}}\sqrt{1-x_3^2} - x_3\sqrt{1-\frac{a^2}{1-x_1^2}} = 0 \tag{7'}$$

$$fx_3 + \sqrt{1 - \frac{f^2}{1 - x_1^2}} \sqrt{1 - x_3^2} = 0 \tag{8'}$$

$$ac + \frac{-ax_1}{\sqrt{1 - x_1^2}} \frac{-cx_1}{\sqrt{1 - x_1^2}} + \sqrt{1 - \frac{a^2}{1 - x_1^2}} \sqrt{1 - \frac{c^2}{1 - x_1^2}} = 0$$
 (9')

$$\frac{fx_1}{\sqrt{1-x_1^2}} \frac{hx_1}{\sqrt{1-x_1^2}} + fh + \sqrt{1 - \frac{f^2}{1-x_1^2}} \sqrt{1 - \frac{h^2}{1-x_1^2}} = 0$$
 (10')

These can then almost trivially be rewritten to:

$$hx_1\sqrt{1-x_2^2} - x_2\sqrt{1-x_1^2 - h^2} = 0 (5")$$

$$cx_2\sqrt{1-x_1^2} + \sqrt{1-x_2^2}\sqrt{1-x_1^2-c^2} = 0 (6")$$

$$ax_1\sqrt{1-x_3^2} + x_3\sqrt{1-x_1^2-a^2} = 0 (7")$$

$$fx_3\sqrt{1-x_1^2} + \sqrt{1-x_1^2 - f^2}\sqrt{1-x_3^2} = 0$$
 (8")

$$ac + \sqrt{1 - x_1^2 - a^2} \sqrt{1 - x_1^2 - c^2} = 0$$
 (9")

$$fh + \sqrt{1 - x_1^2 - f^2} \sqrt{1 - x_1^2 - h^2} = 0 \tag{10}$$

It then follows from (7"), (9") and (6") that:

$$\frac{\sqrt{1-x_3^2}}{x_3} = \frac{-\sqrt{1-x_1^2-a^2}}{ax_1}$$
$$= \frac{c}{x_1\sqrt{1-x_1^2-c^2}}$$
$$= \frac{-\sqrt{1-x_2^2}}{x_1x_2\sqrt{1-x_1^2}}$$

While using (5"),(10") and (8") we find that:

$$\frac{\sqrt{1-x_2^2}}{x_2} = \frac{\sqrt{1-x_1^2-h^2}}{hx_1}$$

$$= \frac{-f}{x_1\sqrt{1-x_1^2-f^2}}$$

$$= \frac{\sqrt{1-x_3^2}}{x_1x_3\sqrt{1-x_1^2}}$$

Inserting this expression for $\frac{\sqrt{1-{x_2}^2}}{x_2}$ into the expression for $\frac{\sqrt{1-{x_3}^2}}{x_3}$ we obtain the equation:

$$\frac{\sqrt{1-x_3^2}}{x_3} = \frac{-\sqrt{1-x_3^2}}{x_3x_1^2(1-x_1^2)} \tag{12}$$

But then, eliminating the x_3 terms we find:

$$x_1^2(1-x_1^2) = -1 (13)$$

Which is our desired contradiction.

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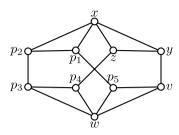
Appendix B: Second Cross-product Unembeddability Proof

Proposition B.1

The graph on the right is not embeddable.

Proof

Suppose it is embeddable. Note (the point associated to) p_5 is orthogonal to (the points associated to) v and w. As $v \neq w$, we see p_5 is collinear to cross-product $v \times w$. Similarly, we derive



$$p_1 \text{ coll. } x \times (v \times w)$$
 $p_4 \text{ coll. } w \times z$
 $p_2 \text{ coll. } x \times (x \times v \times w)$ $p_3 \text{ coll. } w \times (w \times z)$
 $p_3 \text{ coll. } (w \times z) \times (x \times (x \times (v \times w)))$

And thus

$$(w \times (w \times z)) \times ((w \times z) \times (x \times (x \times (v \times w)))) = 0. \tag{14}$$

By rotating the embedding, we may assume without loss of generality that we have z = (0, 0, 1), y = (0, 1, 0) and x = (1, 0, 0). Write

$$v = (v_1, 0, \sqrt{1 - v_1^2})$$
 $w = (w_1, w_2, \sqrt{1 - w_1^2 - w_2^2}).$

Now, equation 14 becomes

$$w_2^2 \left(v_1 - \sqrt{1 - v_1^2} w_1 \sqrt{1 - w_1^2 - w_2^2} \right) = 0$$

$$w_1 w_2 \left(\sqrt{1 - v_1^2} w_1 \sqrt{1 - w_1^2 - w_2^2} - v_1 \right) = 0.$$

Note $w_1 \neq 0$, for otherwise w would be orthogonal to x, which would imply w = y, quod non. Similarly $w_2 \neq 0$, for otherwise w would be orthogonal to y and then $v = p_4$, quod non. And finally, $v_1 \neq 0$, for otherwise v would be orthogonal to x and then $x = p_5$, quod non. It follows

$$v_1 = \sqrt{1 - v_1^2} w_1 \sqrt{1 - w_1^2 - w_2^2}.$$

As v is orthogonal to w, we have $-v_1w_1 = \sqrt{1-v_1^2}\sqrt{1-w_1^2-w_2^2}$. Substituting this in the previous equation, we get $v_1 = -v_1w_1^2$. That is: $w_1^2 = -1$, which is absurd. Apparently, the graph cannot be embeddable.

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A Kochen-Specker System Has at Least 22 Vectors



Sander Uijlen: He is a Ph.D. student at the Institute for Computing and Information Sciences at the Radboud University in Nijmegen. He has a background in physics and mathematics and currently his main interests are the mathematical structures of contextuality and non-locality.



Bas Westerbaan: He is a Ph. D.-researcher at the Institute for Computing and Information Sciences at Radboud Universiteit Nijmegen. His current research is focused on the categorical properties of operator algebras relevant to the semantics of quantum computers.