Obtaining Massive Data Sets for Contextual Experiments in Quantum Information

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***Abstract*—Finding even the simplest Kochen-Specker sets for contextual experiments—a hot subject in the field of quantum information theory, theoretically and experimentally—by brute force would take all the clusters on Earth more than the Age of Universe. Human ingenuity found about a dozen such sets in the last 40 years. I will present how our group reduced this finding of contextual needles in a haystack to a manageable task, by first visualising them via hypergraphs, human-derived from the space symmetries, and then running jobs that generate the sets—billions of them—in parallel.**

I. Introduction

A measurement of any observable of a classical system should yield the same value independently of whether we carry out the measurement of the observable simultaneously with another measurement of another observable of the same system or not. In other words, classical theories do not depend on arrangements in which measurements are carried out, i.e., on their "context," and we say that classical theories are *non-contextual* and that all their observables can be ascribed predetermined values.

In contrast, a measurement of an observable of a quantum system can yield different values depending on other measurements of another observables that we measure simultaneously with the considered observable. So, a quantum theory does depend on arrangements in which measurements are carried out and we say that quantum theories are *contextual* and that their observables cannot be ascribed predetermined values.

Not all experimental arrangements for a quantum system are contextual, though. Actually, until a few years ago only about a dozen such sets of quantum states to which no predetermined values can be ascribed were known. The sets are called Kochen-Specker (KS) sets and they are needed not only for a better understanding of quantum theories and measurements [1]–[3], but also for constructing of quantum gates in the field of quantum information and quantum computation and for handling quantum sets in general [4], [5]. So, it is of interest to know how often we can encounter such sets, i.e., how many KS sets we can generate.

II. Formalism

Let us first define KS sets more precisely.

Definition 1. Every KS set is a set of vectors in a Hilbert space $\mathcal{H}^n$, $n \geq 3$ to which it is impossible to assign 1's and 0's in such a way that:

1. No two orthogonal vectors are both assigned the value 1;
2. Not all of any mutually orthogonal vectors are assigned the value 0.

In this presentation we shall limit ourselves to $n = 4$, i.e., a 4-dim Hilbert space. Systems can be either a pair of qubits (qubit is a 2-dim quantum system) or a spin-3/2 particles. Sets of mutually orthogonal vectors in a 4-dim space we call tetrads. A KS set is a union of such tetrads.

Mutual orthogonality of 4 vectors in a 4-dim Hilbert space is represented by the following 6 nonlinear equations:

$$
\begin{aligned}
\mathbf{a}_A \cdot \mathbf{a}_B &= a_{A1}a_{B1} + a_{A2}a_{B2} + a_{A3}a_{B3} + a_{A4}a_{B4} = 0,\\
\mathbf{a}_A \cdot \mathbf{a}_C &= a_{A1}a_{C1} + a_{A2}a_{C2} + a_{A3}a_{C3} + a_{A4}a_{C4} = 0,\\
\mathbf{a}_A \cdot \mathbf{a}_D &= a_{A1}a_{D1} + a_{A2}a_{D2} + a_{A3}a_{D3} + a_{A4}a_{D4} = 0,\\
\mathbf{a}_B \cdot \mathbf{a}_C &= a_{B1}a_{C1} + a_{B2}a_{C2} + a_{B3}a_{C3} + a_{B4}a_{C4} = 0,\\
\mathbf{a}_B \cdot \mathbf{a}_D &= a_{B1}a_{D1} + a_{B2}a_{D2} + a_{B3}a_{D3} + a_{B4}a_{D4} = 0,\\
\mathbf{a}_C \cdot \mathbf{a}_D &= a_{C1}a_{D1} + a_{C2}a_{D2} + a_{C3}a_{D3} + a_{C4}a_{D4} = 0.
\end{aligned}
$$

Now, it might seem that the problem can be approached by a brute computational force. We ascribe values 0 and 1 to various sets of connected tetrads of vectors and as soon as we find a set for which we cannot do that it is a KS set. However, this is easier said than done because there are billions of such sets even if we limit ourselves only to unit components along each of four axes for all vectors. Besides, the equations are nonlinear and it is a hard problem with only a few equations, let alone billions.

Fortunately, in 2000 I realised that these equations can be reduced to a generation and then filtering of hypergraphs, in particular McKay-Megill-Pavičić (MMP) hypergraphs, which Brendan D. McKay, Norman D. Megill, and I defined previously for another purpose.

Definition 2. We define MMP hypergraphs as follows [6]

(i) Every vertex belongs to at least one edge;
(ii) Every edge contains at least 3 vertices;
(iii) Edges that intersect each other in $n - 2$ vertices contain at least n vertices.

This definition enables us to formulate algorithms for exhaustive generation of MMP hypergraphs. In this work we shall work with subsets of a 60-75 (60 vertices - 75 edges) master set obtained by P. K. Aravind who derived it from another even bigger set using geometric symmetries [7]. From this master set we generate smaller hypergraphs that correspond to subsets of the 60-75 set with a specified number of edges deleted.

For any experimental application it is not viable to consider all KS (sub)sets but only those that can be experimentally distinguished. Hence, we extract *critical* non-redundant non-isomorphic KS sets. "Critical" means that they are minimal in the sense that no orthogonal tetrads can be removed without causing the KS contradiction to disappear.

The "only" difficulty we face is the sheer size of these generated subsets—we are dealing with a haystack of 2^{75} or 38 sextillion subsets, in which we wish to find certain "needles," i.e., critical KS sets. In Sec. III we will present the algorithms and programs which enable us to deal with the haystack.

The hypergraphs we obtain reflect only the orthogonal structure of KS sets and do not in any way refer to the vector components of the original 60-75 KS set. This is yet another aspect in which the present method differs from the parity-proof method we used in [8], which relies on the vector components of the vectors in each KS set that were inherited from the original 60-75 set. For each hypergraph we can, however, find appropriate vector components with our program `vectorfind` or by interval analysis we developed in [6].

We encode MMP hypergraphs by means of alphanumeric and other printable ASCII characters. Each vertex is represented by one of the following characters: 1 2 3 4 5 6 7 8 9 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z a b c d e f g h i j k l m n o p q r s t u v w x y z ! " # $ % & ' ( ) * - / : ; < = > ? @ [\ ] ^ _ ` { | } ~ , and then again all these characters prefixed by '+', then prefixed by '++', etc.

Each edge is represented by a string of characters that represent vertices within a single line. Edges are separated by commas. The line must end with a full stop. Skipping of characters is allowed. A line forms a representation of a hypergraph. The order of the edges is irrelevant. The numbers of vertices and edges are unlimited. We often present MMP hypergraphs starting with edges forming the biggest loop to facilitate their possible drawing.

In Fig. 1 we show a graphical representation of the minimal (26-13) critical KS set we found and which we shall now use to show a correspondence between the vector and the MMP hypergraph representation of any KS set.

Each vertex represents a vector in a 4-dim space. For instance, G$=\{1,0,0,0\}$, F$=\{0,1,0,0\}$, E$=\{0,0,1,0\}$, D$=\{0,0,0,1\}$. They are mutually orthogonal and that means they form an edge—GFED. Our program `vectorfind` can assign all vectors, that correspond to edges from the 26-13 set, component values from the set $\{0,\pm1,\pm(\sqrt{5}+1)/2,\pm(\sqrt{5}-1)/2\}$ and that means that the system of equations that define all orthogonalities for the 26-13 does have a solution. Now our program `states01` (which exhaustively verifies all possible assignments) checks whether all the vertices can be ascribed 0 and 1 according to the KS rules 1 and 2 above and verifies that it is not possible. The main point here is that we can always go from MMP hypergraphs to vectors and back and that `states01` works with MMP hypergraphs. MMP hypergraphs are linear while the system of equations describing mutual orthogonality of vectors are nonlinear. Therefore the evaluation of MMP hypergraphs by means of `states01` is exponentially faster than solving nonlinear equations and this is what makes our generation of KS sets feasible. While the algorithm used in `states01` is comparatively fast, the verification of KS sets for MMP hypergraphs with an odd number of edges can be

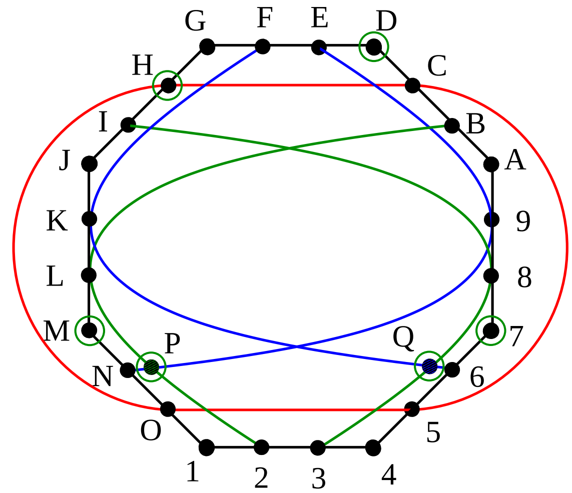


Fig. 1. The smallest KS set 26-13 (with 26 vertices and 13 edges). Possible assignments of 1s are indicated by circles (7,D,H,M,P,Q)—the remaining vertices can only be assigned 0s. Hence, all vertices in edge 1234 can only be assigned 0s and Def. 1 is satisfied. MMP encoding of the shown 26-13 reads: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNO1,O5CH,2PLB,NP9E,6FQK,3Q8I..

even faster using our "parity proofs" algorithm described in [8].

We stress here that once we visualised, i.e., drew, MMP hypergraphs, we can drop the ASCII signs and compare and classify them graphically referring only to, e.g., the biggest loops they allow, the highest and lowest numbers of edges vertices allow, whether they allow parity proofs, the highest number of 1s vertices can be assigned, etc., all of which properties have their own role in experimental implementation of critical KS sets. Of course, we can always go back to vector representation so as to assign arbitrary ASCII signs to vertices and then run `vectorfind` on them.

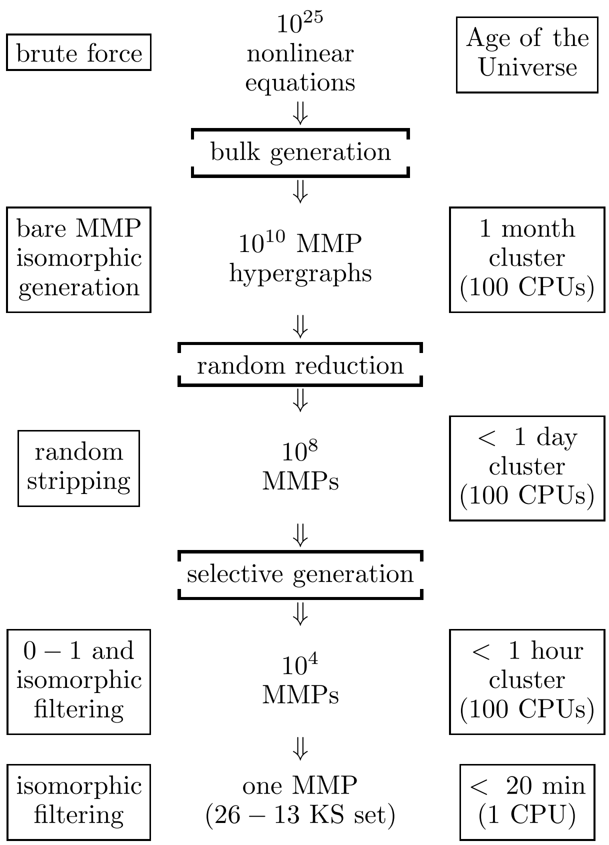
III. Results

To generate critical KS sets we applied an algorithm and a program (`mmpstrip`) which strip edges from the master 60-75 MMP, then subsequently from the so obtained MMPs, and so on. The number of MMPs we can obtain in this way grows exponentially and in less then 10 steps it would make busy all CPUs and would overflow all storage capacities on the Globe.

Fortunately the greatest portion of the generated MMPs are isomorphic to each other and by using B. D. McKay's algorithm and program `shortd` which he derived from his program `nauty`, we are able to greatly reduce the number of MMPs we have to generate to eventually obtain the required critical KS sets. However, even their number is far too big for an exhaustive generation and even clusters with hundreds of CPUs cannot make more than 13 steps in an acceptable time.

Therefore the only option left is a probabilistic generation combined with 0-1 and isomorphic filtering. That excludes parallel processing on a cluster because the programs for stripping, isomorphic reduction, and 0-1 filtering are all probabilistic so far as the sequential steps are concerned (although, of course, the end result is deterministic). Thus the times of parallel running greatly differ and it is much more efficient to put a large number of jobs in queue and rerun those that come out first. The details are as follows.

As shown in the flowchart 1, we first have to generate—by stripping edges—a sufficient number of MMPs, in several steps, to compensate for an inherent homogeneous distribution of critical MMPs in the generation "down-tree." After each step, i.e., with a sufficient number of MMPs within each step, we reiterate the procedure until we reach about " 10^{10} MMPs. Then we carry out a "random reduction" by means of `states01` which strips random edges from the input MMPs until they are critical.



(1)

The majority of so obtained criticals are isomorphic and mixed. Therefore we have to rerun the random reduction and selective generation many times and each time we have to merge new MMPs with the already obtained ones so as to build a cumulative set of all possible KS. However, not even then can we be sure that we obtained samples of all kinds of MMPs. For example, after 3500 generated 60-41 critical MMPs (critical KS sets) among more than 1.5 billion critical KS sets we still have not obtained a single one with a parity proof although there is at least one because we obtained it via a parity algorithm from [8]. On the other hand a single 47-30 appeared only after 1 billion of generated KS criticals and it cannot be generated via the parity algorithm since it has an even number of edges. We present statistics of obtained critical KS sets in Fig. 2. Detailed presentation of all obtained results will appear in a subsequent publication.

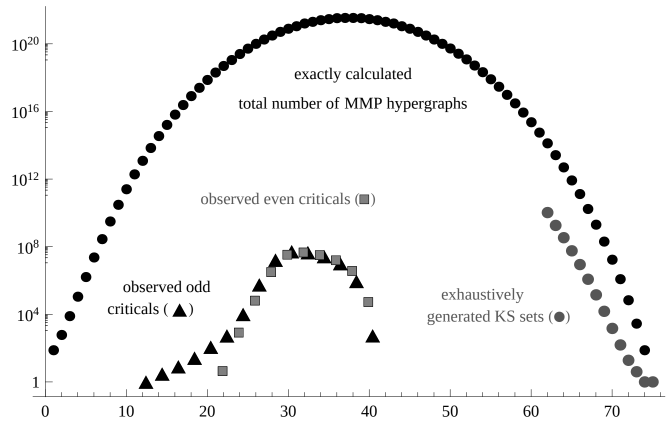


Fig. 2. Statistics calculated for subsets of 60-75 given on a logarithmic scale. There are more than 10^9 critical KS sets. Given numbers of critical KS sets with 13 to 27 edges (on the x-axis) are exhaustive. The number of criticals with 32 edges is the biggest; we estimate that they do not exceed 10^{10}. Given numbers of noncritical KS sets with more than 61 edges are also exhaustive.

Details of the programs `mmpstrip`, `states01`, `vectorfind`, and `shortd` and the algorithms behind them are given in [6]–[9].

IV. Conclusion

We have obtained a massive number of contextual sets, more specifically critical Kochen-Specker (KS) sets, by first translating a condition imposed on quantum states—orthogonality—into a condition imposed on correlated MMP hypergraphs and then handling the latter hypergraphs to generate the sets. In the standard Hilbert space the generation lead to huge sets of nonlinear equations and therefore to an exponentially complex problem. Generation of MMP hypergraphs is however a statistically polynomial problem and is therefore feasible, although lengthy as shown in the previous section. "Statistically polynomial" here means that although the algorithms behind the programs `mmpstrip` and `states01` might in general take an exponentially increasing time with larger sets, this on average does not happen because of the inner structure of the KS sets.

Obtaining large KS sets is important for better understanding of how quantum system behave and a better insight into their engineering within experiments. The most significant result we obtained is that efficiency of contextual measurements does not drop with large KS sets. Only the number of required measurement rises but the efficiency of each of them can be the same for some of the largest sets as for the smallest one. This is in contrast with most other quantum gates where the efficiency drops when the number of states increases, due to coherence problems. On the other hand, some of our previous conjectures based on a smaller number of sets [9] should be amended. For instance, the peak for the KS criticals turn out to be much lower, the distribution of them of a different shape, and the KS criticals with more than 41 edges nonexistent.

Also a very important contribution of a computational approach to contextual sets and similar problems is contained in our development of algorithms that enable solving huge systems of nonlinear equations via handling MMP hypergraphs on clusters. This is important not only because we already arrived at new results with new KS sets in 3-, 4-, and 6-dim Hilbert spaces, but also because it opens a new approach to solving systems of equations in an analogous way in other quantum and classical problems—whenever we can translate a condition imposed on a system of equations into a condition imposed on hypergraphs, we should be able to solve the system via handling and filtering the hypergraphs.

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