Notes on Contextuality

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1 Introduction

To do.

2 Fundamentals

Suppose we can perform on a system measurements of some observables $A_1, A_2, \dots, A_n$, whose outcomes are designated by $a_1, a_2, \dots, a_n$, and suppose that not all of these observables can be measured at once without disturbing the system. We call the properties that can be measured together *compatible*, and *non compatible* the ones that cannot.

We then define as the *context* of the measurement of A_i the other *compatible* properties that are measured together with it. A theory is said to be *non contextual* if the predicted outcome a_i of some observable A_i does not depend on the context. If it does we say that the theory is *contextual*.

In quantum theory compatible measurements are represented by commuting operators on a Hilbert space $\mathcal{H}$. In this section we can limit ourselves to consider only dichotomous measurements, which are represented by projectors in QM. Compatible observables in this case are equivalent to orthogonal projectors.

In QM contextuality is said to be *not explicit*. This means that the outcome of a measure of an observable A_i may depend on the context, but the probability for that single observable $p(A_i = a_i)$, does not. This is also called the *no-disturbance* or *no-signaling* principle.

Nonetheless, as we will show in this section, a non-contextual HVT (hidden variable theory) cannot reproduce the prediction of QM.

2.1 Joint probability

The problem of the existence of a non-contextual HVT can be better expressed in terms of probability distributions. To simplify the notation we call $f(a_1, \dots, a_k) = p(A_1 = a_1, \dots, A_k = a_k)$ the probability that the measure of $A_1, \dots, A_k$ gives outcomes $a_1, \dots, a_k$.

Quantum mechanics gives us only the joint probability distribution for *compatible* observables. So if $\{A_1, A_2\}$ are compatible observables, but $\{A_1, A_2, A_3\}$ are not, QM gives us only $f(a_1, a_2)$, without any information about an hypothetical $f(a_1, a_2, a_3)$.

A non-contextual HVT instead, the presence of a global joint probability distribution for all observables $f(a_1, \dots, a_n)$ is assured by the fact that every property of the system must have a definite value, and the uncertainty is only given by our ignorance about the initial conditions. From that global joint distribution one should be able to derive the quantum mechanical ones for compatible observables $f(a_1, \ldots, a_k)$, as marginals.

The possibility of the existence of a joint probability distribution depends on the compatibility relations between the observables. To better visualize them, we can construct a graph where every vertex represents an observable and two vertex are connected if the corresponding observables are compatible, some examples are shown in figure 1.

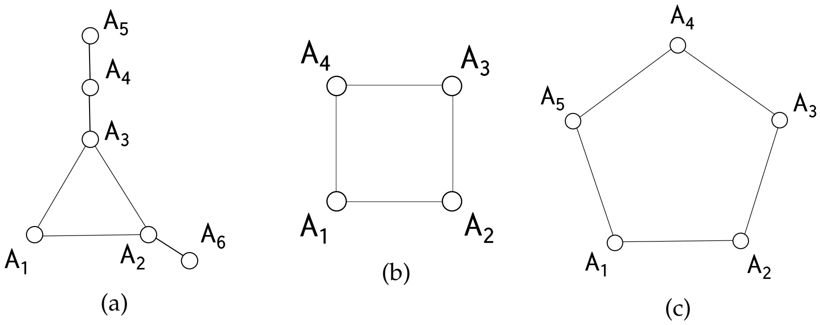


Figure 1: Examples of compatibility graphs

A sufficient condition for the existence of a joint probability distribution is that the corresponding graph should not contain *n-cycles* with $n > 3$. [1] This statement is easily proved by constructing the joint probability for such a graph.

Proof. If there are only 3-cycles, it is always possible to construct a global joint probability distribution from the joint distributions of compatible observables as follows: first multiply together the joint distribution for every 3-cycle [2] $f(a_i, a_j, a_k)$, then multiply those by the joint distributions for all the other edges, and if an observable is present in more than one distribution divide by $f(a_l)^{n-1}$, where n is the number of terms in which it appears. For example, for the first graph in figure 1 we have:

$$f(a_1, \ldots, a_6) = \frac{f(a_1, a_2, a_3) f(a_2, a_6) f(a_3, a_4) f(a_4, a_5)}{f(a_2) f(a_3) f(a_4)}$$

from which all the joint distributions for every edge can be obtained by summing over the other variables. $\square$

So for example it is certainly possible to construct such a distribution for graph 1a, but not for graphs 1b and 1c.

While this gives no information about the existence of a joint distribution for other graphs, the next two theorems will prove that a similar construction is impossible in general.

[1]The definition of *n-cycle*, and other terms related to graph theory, is given in the appendix A.

2.2 Gleason's theorem

In the course of an analysis on the axioms of quantum theory, Gleason proved an important theorem that poses a limit to form that the distribution of an hypothetical HVT could have.

As we said in quantum theory every yes-no test about a system can be represented by a projector $\mathbf{P}$ in a Hilbert space $\mathcal{H}$. A *quantum probability distribution* is a function $f(\mathbf{P})$ that assign to every such projector a value such that:

$$f(\mathbf{P}) > 0$$
$$\sum_i f(\mathbf{P}_i) = 1 \qquad \text{for every orthogonal base} \quad \{P_i\}$$

What Gleason proved is that every quantum probability distribution f on an Hilbert space of dimension greater than three can be written as:

$$f(\mathbf{P}) = \mathrm{Tr}(\rho\mathbf{P}) \tag{1}$$

for a suitable positive semi-definite, hermitian operator ρ, such that $\mathrm{Tr}(\rho) = 1$. This means that the density matrix formalism is enough to describe the most general kind of quantum probability distribution in an Hilbert space.

Proof. To do. $\square$

With this theorem is possible to deduce quantum theory from these three postulates:

1. Dichotomous tests are represented by projectors in a Hilbert space.
2. Compatible test are represented by commuting projectors.
3. If P and Q are orthogonal projector then

$$\langle P + Q \rangle = \langle P \rangle + \langle Q \rangle$$

For a non-contextual HVT to exist, it has to be possible then to define a function $f(P)$ with values 0 or 1 for every projector P in $\mathcal{H}$. Such a function cannot be written in the form (1), required by Gleason theorem for a probability distribution in $\mathcal{H}$, so for a HVT, we are forced to abandon axiom (3).

2.3 Kochen-Specker theorem

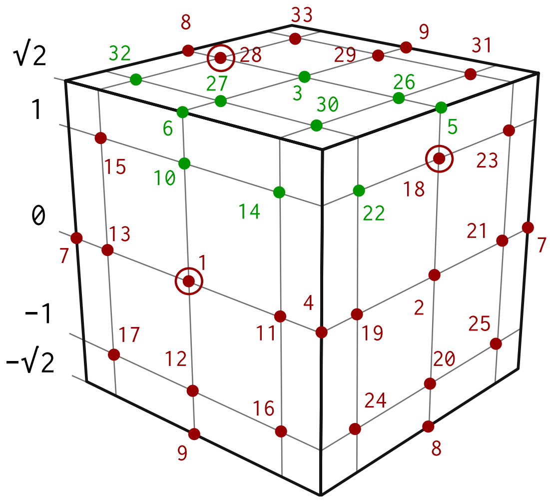
This fundamental incompatibility is better expressed by the Kochen-Specker theorem.

This theorem affirms that in an Hilbert space $\mathcal{H}$ of dimension $d \geqslant 3$, there is no function h from the set of projectors of $\mathcal{H}$ to $\{0, 1\}$ such that:

$$\sum_i P_i = \mathbf{I} \implies \sum_i h(P_i) = 1 \tag{2}$$

The proofs of this theorem are usually constructive: they present a set of projectors and show how such a function h cannot be defined. The original proof used 117 projectors in a three dimensional space, but smaller sets exists. For example this proof, due to A. Peres uses only 33 rays:

Proof. The 33 rays in question are shown in figure and listed in the table below. We will show that is impossible to assign value 1 or 0 to these rays without violating (2). To better visualize the argument we will use the colors *green* and *red* to represent the values 1 and 0 respectively.



Peres KS set

1	$(1,0,0)$	12	$(\sqrt{2},0,-1)$	23	$(-1,\sqrt{2},1)$
2	$(0,1,0)$	13	$(\sqrt{2},-1,0)$	24	$(1,\sqrt{2},-1)$
3	$(0,0,1)$	14	$(\sqrt{2},1,1)$	25	$(-1,\sqrt{2},-1)$
4	$(1,1,0)$	15	$(\sqrt{2},-1,1)$	26	$(0,1,\sqrt{2})$
5	$(0,1,1)$	16	$(\sqrt{2},1,-1)$	27	$(1,0,\sqrt{2})$
6	$(1,0,1)$	17	$(\sqrt{2},-1,-1)$	28	$(0,-1,\sqrt{2})$
7	$(-1,1,0)$	18	$(0,\sqrt{2},1)$	29	$(-1,0,\sqrt{2})$
8	$(0,-1,1)$	19	$(1,\sqrt{2},0)$	30	$(1,1,\sqrt{2})$
9	$(1,0,-1)$	20	$(0,\sqrt{2},-1)$	31	$(-1,1,\sqrt{2})$
10	$(\sqrt{2},0,1)$	21	$(-1,\sqrt{2},0)$	32	$(1,-1,\sqrt{2})$
11	$(\sqrt{2},1,0)$	22	$(1,\sqrt{2},1)$	33	$(-1,-1,\sqrt{2})$

As we can see the system is symmetric under the interchange or the reversal of the axes x, y, z. This means that without losing generality we can paint green any of the rays in the orthogonal triad $\{1,2,3\}$. Similarly in $\{1,5,8\}$ we can choose between 5 or 8 (reversal of the y axis), between 6 or 9 in $\{2,6,9\}$ (reversal of the x axis) and between 31 or 32 in $\{4,31,32\}$ (interchange of x with y).

If we choose for example to paint 3, 5, 6 and 32 green, the value of the other rays will be fixed by the procedure shown below:

$$
\begin{array}{lllll}
3 & \Longrightarrow & 1,2,4,7,11,13,19,21 & & \\
5 & \Longrightarrow & 1,8,15,16 & & \\
6 & \Longrightarrow & 2,9,23,24 & & \\
32 & \Longrightarrow & 4,12,18,31 & & \\
\hline
12,2 & \Longrightarrow & 27 & \Longrightarrow & 17 \\
8,17 & \Longrightarrow & 14 & \Longrightarrow & 29 \\
29,2 & \Longrightarrow & 10 & \Longrightarrow & 33 \\
33,7 & \Longrightarrow & 30 & \Longrightarrow & 20 \\
20,1 & \Longrightarrow & 26 & \Longrightarrow & 25 \\
25,8 & \Longrightarrow & 22 & \Longrightarrow & 28
\end{array}
$$

But with this coloring the rays $\{1, 18, 28\}$, which form an orthogonal triad, are all red: we have a contradiction, and since the initial assignments where completely general the theorem is proved. □

Clearly this means that an HVT, that assigns definite values 0 or 1 to every yes-no test regardless of the context, is fundamentally incompatible with QM. In fact every such assignment has to satisfy (2), since a set of projectors that sums to identity represent a complete test, so the assigned values must sum to unity. But we have just that proved that this is not possible in general for $d \geqslant 3$.

Other kinds of proofs exists which relies on general observables (not just projectors), like the Peres-Mermin square described in 3.3, or on inequalities as shown in 3.4.

2.4 Experimental Test of KS theorem

What we have shown is just that the QM predictions are impossible to reproduce with a classically behaving HVT. The next obvious step would be to see which way nature prefers by testing it experimentally. While it is possible to test the Kochen-Specker directly using the proof presented in the last section (or other equivalent proofs), this approach is known to be problematic.

One of the biggest problem is that every observable must be measured in more than one, incompatible contexts. So one could not discard the possibility that the results are influenced by the different measurement's procedure. The inequalities, described in the next section, offer a better alternative for experimental verification.

Another difficulty lies in the precision with which we can measure an observable: there is always the chance that our measured observable could differ slightly from the one we wanted to measure, this is called the *finite precision problem*. Since it can be shown that it is possible to approximate a KS set of rays with a non KS one, this is a serious problem in testing the KS theorem. The way out of it is to create new versions of the KS theorem for imprecisely defined observables, often expressed as the already mentioned inequalities.

The impossibility to precisely define an observable leads also to the *problem of compatibility*: we cannot assume that the observable are compatible anymore, and as we have seen, this is a crucial assumption for testing contextuality. To deal with this problem, we need to add new terms to the classical bound in inequalities, as will be described in the next section.

3 Non-contextual inequalities

In some systems, assuming classical behavior implies that certain combinations of correlations between observables are bounded by an inequality that is violated QM. This suggests another way to prove and to test the fundamental incompatibility between QM and non-contextual theories.

The most famous of these inequality is certainly the *Bell theorem*, which showed how QM cannot be described by a local HVT. Since non-locality is a particular form of contextuality, the same inequality can be used to settle the question of the existence of non-contextual HVT, and is described in section 3.1 (in the form of the CHSH inequality).

Anyway, in the more general setting of contextuality we don't necessarily need two subsystems or entanglement, as we showed in the KS theorem, a spin-1 system is enough.

It is useful to divide non-contextual inequalities into two classes:

- *State-dependent*, where the inequality is violated only when the system is in some particular state.
- *State-independent*, where the inequality is always violated regardless of the state of the system.

Usually state-dependent tests involve less measurements, but obviously need a fixed initial state, while state-independent does not.

As in section 2.1, we can associate a graph to every non-contextual inequality. There are two ways to construct a graph for an inequality test:

- The *Compatibility graph* is the graph constructed from the set of observables: in such a graph every observable is represented by a vertex and two vertex are connected if the corresponding observables are compatible.
- The *Exclusivity graph* constructed from the single dichotomous exclusive events, where every vertex represent a yes-no measurement (a projector in the quantum formalism), and edges represent exclusivity (orthogonality in QM).

In the next sections we will describe some of the most common non-contextual inequalities.

3.1 CHSH

This inequality was first devised by Clauser, Horne, Shimony and Holt as an alternative to the Bell inequality to test non-locality. For this reason the system is composed by two 2-dimensional subsystems (normally spin-$\frac{1}{2}$ particles) in entanglement, that can be separated by a space-like distance.

The experimenters can measure the spin on their particles in two different directions. The chosen observable are:

$$
\begin{aligned}
A_1 &= \sigma_x \otimes \mathbf{I} & \qquad B_1 &= \sigma_z \otimes \mathbf{I} \\
A_2 &= -\mathbf{I} \otimes \frac{\sigma_z + \sigma_x}{\sqrt{2}} & \qquad B_2 &= \mathbf{I} \otimes \frac{\sigma_z - \sigma_x}{\sqrt{2}}
\end{aligned}
$$

and the corresponding compatibility graph is shown in figure 2a.

Since the observables measured can takes only ± 1 values if we suppose a classical, non-contextual(or local) behavior we expect:

$$\langle (A_1 + B_1)A_2 + (B_1 - A_1)B_2 \rangle = \langle A_1A_2 + B_1A_2 + B_1B_2 - A_1B_2 \rangle \leqslant 2 \qquad (3)$$

But if, say, we prepare the system in the entangled state

$$|\psi\rangle = \frac{|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle}{\sqrt{2}}$$

QM predicts:

$$\langle A_1A_2 \rangle + \langle B_1A_2 \rangle + \langle B_1B_2 \rangle - \langle A_1B_2 \rangle = 2\sqrt{2}$$

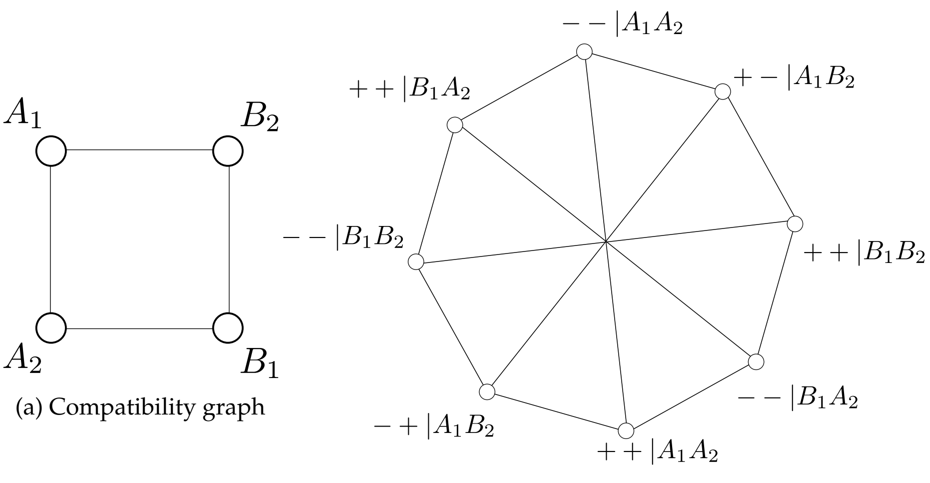
so (3) is violated by quantum mechanics. Notice that for the inequality to be violated the system has to be in a particular entangled state, so this is an example of a state-dependent inequality.

We can also write (3) using directly probabilities for exclusive events:

$$\begin{aligned} & p(11|A_1A_2) + p(-1-1|A_1A_2) + p(11|B_1B_2) + p(-1-1|B_1B_2) + \\ & \qquad p(11|B_1A_2) + p(-1-1|B_1A_2) + p(-11|A_1B_2) + p(1-1|A_1B_2) \leqslant 3 \end{aligned}$$

where $p(ab|AB)$ represents the probability of having oucomes a and b measuring the properties A and B. The events involved are represented in the exclusivity graph 2b.

It can be shown that in QM the maximum value of this sum is $2 + \sqrt{2}$, so the inequality is again violated.



(a) Compatibility graph

(b) Exclusivity graph

Figure 2: Graphs for the CHSH inequality

3.2 KCBS

A more recent example of a state-dependent non-contextual inequality is called the KCBS inequality, from Klyachko, Can, Binicioglu and Shumovsky.

Here we have a 3-dimensional system (like a spin-1 particle), and five dichotomous observables which can take values $\{0,1\}$ and satisfy the exclusivity relations shown in figure 3. For example this can be implemented measuring

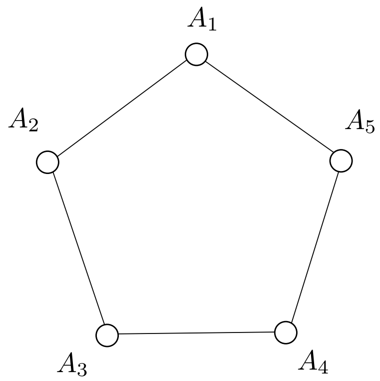


Figure 3: Exclusivity graph for the *KCBS* inequality

$A_i = 1 - S_i^2$, where the S_i are the spin observables for a spin-1 particle in five different direction.

Classically, since only 2 observables can be assigned the value 1 to satisfy the exclusivity graph, we have the inequality.

$$\sum_{i=1}^{5} a_i \leqslant 2 \tag{4}$$

This inequality is often presented in another form, using the observables $B_i = 2A_i - 1$ instead that takes the values $\{1, -1\}$, so that (4) becomes:

$$\langle B_1 B_2 \rangle + \langle B_2 B_3 \rangle + \langle B_3 B_4 \rangle + \langle B_4 B_5 \rangle + \langle B_5 B_1 \rangle \geqslant -3 \tag{5}$$

In QM the $A_i = |a_i\rangle \langle a_i|$ are projectors in a 3-dimensional Hilbert space, with orthogonality relations given by the graph 3. For example we can use the rays:

$$\begin{aligned}
|a_1\rangle &= \left(1, 0, \sqrt{\cos(\pi/5)}\right) \\
|a_2\rangle &= \left(-\cos(\pi/5), \sin(\pi/5), \sqrt{\cos(\pi/5)}\right) \\
|a_3\rangle &= \left(-\cos(\pi/5), -\sin(\pi/5), \sqrt{\cos(\pi/5)}\right) \\
|a_4\rangle &= \left(-\cos(2\pi/5), \sin(2\pi/5), \sqrt{\cos(\pi/5)}\right) \\
|a_4\rangle &= \left(-\cos(2\pi/5), -\sin(2\pi/5), \sqrt{\cos(\pi/5)}\right)
\end{aligned}$$

directed along the vertices of a pentagram. If we measure them on the state $|\psi\rangle = (1, 0, 0)$ we have

$$\sum_{i=1}^{5} |\langle a_i \,|\, \psi\rangle|^2 = \sqrt{5} > 2$$

which correspond to a violation of $5 - 4\sqrt{5}$ for the inequality (5).

3.3 Peres-Mermin square

This state-independent inequality has its origin in another proof of the Kochen-Specker theorem.

Suppose to have a system similar to the one used for the CHSH inequality: two particles of spin-$\frac{1}{2}$, and consider the observables:

$$\begin{array}{lll} A_{11} = \mathbf{I} \otimes \sigma_z & A_{12} = \sigma_z \otimes \mathbf{I} & A_{13} = \sigma_z \otimes \sigma_z \\ A_{21} = \sigma_x \otimes \mathbf{I} & A_{22} = \mathbf{I} \otimes \sigma_x & A_{23} = \sigma_x \otimes \sigma_x \\ A_{31} = \sigma_x \otimes \sigma_z & A_{32} = \sigma_z \otimes \sigma_x & A_{33} = \sigma_y \otimes \sigma_y \end{array} \tag{6}$$

The last element of every row is the product of the other two, and the same is true for the columns, except for the last one since:

$$(\sigma_z \otimes \sigma_z)(\sigma_x \otimes \sigma_x) = -\sigma_y \otimes \sigma_y$$

For this reason a fixed assignment of values $\{1, -1\}$ to every observable in (6) is not possible, and this rules out the possibility of having a non-contextual HVT to explain those measures.

This can also be rephrased in the form of an inequality:

$$\begin{aligned} &\langle A_{11}A_{12}A_{13}\rangle + \langle A_{21}A_{22}A_{23}\rangle + \langle A_{31}A_{32}A_{33}\rangle + \\ &\qquad + \langle A_{11}A_{21}A_{31}\rangle + \langle A_{12}A_{22}A_{32}\rangle - \langle A_{13}A_{23}A_{33}\rangle \leqslant 4 \end{aligned}$$

Which holds classically, since the third element in every correlation is the product of the other two.

But in QM we have:

$$\begin{aligned} &\langle A_{11}A_{12}A_{13}\rangle + \langle A_{21}A_{22}A_{23}\rangle + \langle A_{31}A_{32}A_{33}\rangle + \\ &\qquad + \langle A_{11}A_{21}A_{31}\rangle + \langle A_{12}A_{22}A_{32}\rangle - \langle A_{13}A_{23}A_{33}\rangle = 6 \end{aligned}$$

so the inequality (3.3) is violated for every state of the system.

3.4 Yu-Oh's 13 rays inequality(TODO)

Todo.

3.5 Graph theoretical approach (TODO)

The *exclusivity* graph is a powerful instrument to analyze inequalities. In fact from the graph, we can easily deduce if the inequality is violated by QM, and how much is the violation, as is shown in the next theorems.

Theorem 3.1. *Given a graph G associated with a non-contextual inequality S, the maximum value attainable by a non-contextual HVT is equivalent to the independence number $\alpha(G)$ of the graph while the maximum for quantum theory is the Lovatzs number $\theta(G)$ of the graph, and*

$$\alpha(G) \leqslant \theta(G)$$

Proof. To do. ∎

Theorem 3.2. *The inequality associated with the graph* G *is violated if and only if* G *contain as a subgraph a cycle of* $n \geqslant 5$ *or its complement.*

Proof. To do. ∎

A Basic notions of graph theory(TODO)

Todo In this small section we define all the terms connected to graph theory used in the text.

Definition A.1 (Graph)**.** A graph is a collection of vertex and edges, where every edge connects two vertex.

Kinds of graphs (cycles, complete graphs, etc. . .)

Definition A.2 (Subgraph)**.**

Definition A.3 (Clique)**.**

Definition A.4 (Independence number)**.**

Definition A.5 (Lovatzs number)**.**