A new look at the Kochen-Specker theorem — emergence of completeness

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Kochen-Specker theorem states that exclusive and complete deterministic outcome assignments are impossible for certain sets of measurements, called Kochen-Specker (KS) sets. A straightforward consequence is that KS sets do not have joint probability distributions because no set of joint outcomes over such distribution can be constructed. However, we show it is possible to construct a joint quasi-probability distribution over any KS set by relaxing the completeness assumption. Interestingly, completeness is still observable at the level of measurable marginal probability distributions. This suggests the observable completeness might not be a fundamental feature, but an emergent phenomenon.

I. INTRODUCTION

Violations of Bell inequalities [1, 2], or non-contextuality inequalities [3, 4], imply a lack of a joint probability distribution (JPD) over a set of corresponding measurements [5, 6]. Let us consider one of the simplest examples – the Wright/Klyachko-Can-Binicoglu-Shumovsky (Wright/KCBS) inequality [7, 8]

$$\sum_{i=1}^{5} \langle A_i \rangle \leq 2.$$  \hspace{1cm} (1)

It involves five events, to which one assigns a binary \{0, 1\} random variable (measurement) \{A_i\}_{i=1}^5. The events are cyclically exclusive, i.e., if \(A_i = 1\), then \(A_{i+1} = 0\) (summing is \(\mod 5\)). Moreover, these events are cyclically co-measurable, meaning \(A_i\) can be jointly measured with \(A_{i\pm 1}\), but not with \(A_{i\pm 2}\). The Wright/KCBS scenario can be implemented on a quantum three-level system (qutrit), in which case \(\{A_i\}_{i=1}^5\) are cyclically orthogonal projective rank one measurements. If the qutrit is in a maximally mixed state \(\rho = \frac{1}{3}\), then Tr\(\rho A_i\) = 1/3 for all \(i\) and the inequality (1) is not violated. In this case there exists a classical JPD

$$p(A_1 = a_1, \ldots, A_5 = a_5) \equiv p(a_1, \ldots, a_5),$$  \hspace{1cm} (2)

where \(a_i \in \{0, 1\}\). It recovers all measurable marginal probabilities \(p(a_i, a_{i\pm 1})\). Such a JPD is not unique so here is an example:

\begin{align*}
p(1, 0, 0, 1, 0) & = 1/6, \\
p(1, 0, 0, 1, 0) & = 1/6, \\
p(0, 1, 0, 1, 0) & = 1/6, \\
p(0, 1, 0, 1, 0) & = 1/6, \\
p(0, 0, 1, 0, 1) & = 1/6, \\
p(0, 0, 0, 0, 0) & = 1/6.  \hspace{1cm} (3)
\end{align*}

This JPD obeys the exclusivity relations – no two jointly measurable properties are both assigned the value one. On the other hand, there exists a set of measurements and a qutrit state \(|\psi\rangle\) such that \(|\langle \psi | A_i |\psi\rangle = 1/\sqrt{5}\) for all \(i\) [8]. These measurements violate (1) up to \(\sqrt{5}\), excluding a positive JPD emulation. However, a quasi-probability distribution with negative probabilities (JQD) is possible [9–11], for instance:

\begin{align*}
g(0, 0, 0, 0, 0) & = 1/2\sqrt{5}, \\
g(1, 0, 0, 1, 0) & = 1/2\sqrt{5}, \\
g(0, 0, 1, 0, 1) & = 1/2\sqrt{5}, \\
g(0, 0, 0, 0, 0) & = 1 - 5/2\sqrt{5} \approx -0.118  \hspace{1cm} (4)
\end{align*}

does the job. It satisfies the exclusivity relations and recovers the measurable marginal probability distributions.

Although seemingly exotic, JQD is a well defined mathematical concept [12–14], extensively used in quantum theory since Wigner function discovery [15–19]. Recently we demonstrated that JQDs can also be used as a computational resource to reach a non-classical computing speedup [20]. In addition, the JQD’s negativity can be used as a measure of non-classicality (‘quantumness’) [21–23], hence the Wright/KCBS scenario classifies the maximally mixed state as classical and \(|\psi\rangle\) as non-classical.

Curiously, there are measurement scenarios, contextual for any quantum state [3], called state-independent contextuality (SIC) [4] as opposed to the previous example of state-dependent contextuality (SDC). Can one construct a JQD for any SIC scenario? An instinctive answer is yes but there is a peculiar problem here. Similarly to JPDs, JQDs assign quasi-probabilities to all measurement events. Each such event corresponds to an outcome assignment to all observables at once. However, most SIC scenarios forbid such assignments (not all, see [25]). The flagship specimen is the Kochen-Specker (KS) theorem [24]. It states that for certain measurement sets, KS
sets, it is impossible to find outcome assignments, satisfying *exclusivity* and *completeness*. Exclusivity means that no two measurement events can be observed at the same time. On the other hand, the completeness of a mutually exclusive event sets means that exactly one of these events will be observed. Formally:

1. **Exclusivity** – for a jointly measurable subset of mutually exclusive events, corresponding to \{A_1, A_2, \ldots, A_m\}, at most one of them will occur at the same time, i.e., only the following outcome assignments \{a_1, a_2, \ldots, a_m\} are allowed: \{0, 0, \ldots, 0\}, \{1, 0, \ldots, 0\}, \{0, 1, \ldots, 0\}, \ldots, \{0, 0, \ldots, 1\}.

2. **Completeness** – for a complete jointly measurable subset of mutually exclusive events, corresponding to \{A_1, A_2, \ldots, A_n\}, exactly one of them will occur, i.e., only the following outcome assignments \{a_1, a_2, \ldots, a_n\} are allowed: \{1, 0, \ldots, 0\}, \{0, 1, \ldots, 0\}, \ldots, \{0, 0, \ldots, 1\}.

For the projective quantum measurements, the mutual exclusivity of projector subsets, \(S_E\), is imposed by their mutual orthogonality, i.e., \(A_i A_j = \delta_{ij} A_i\) for all pairs \(\{A_i, A_j\} \in S_E\). On the other hand, a mutually exclusive subset of projectors \(S_C\) is complete if \(\sum_{A_i \in S_C} A_i = 1\). Finally, note that any complete subset is exclusive and any exclusive subset can be extended to a complete subset \(S_E \subseteq S_C\).

The exclusivity is a necessary ingredient of all contextuality scenarios, both state-dependent and state-independent. On the other hand, as far as we know, the completeness assumption is necessary for all known SIC scenarios. In particular, all known KS sets contain complete subsets. Here we show that it is possible to construct a JQD for any KS set if one relaxes the completeness assumption. Moreover, our constructions are compatible with the quantum theory. These JQDs can be used to model realistic measurements on KS sets, where completeness is observed in the measurable marginal distributions. This strongly suggests that completeness might be an emergent, rather than fundamental phenomenon.

## II. IDEA

Before we show how to construct a JQD for a given KS set, let us present a simple idea of how observable completeness, as well as exclusivity, emerge in quasi-probability theories.

Consider two events \(A\) and \(B\) with attached indicator random variables (indicators), \(R_A\) and \(R_B\). These indicators have outcome one, if the corresponding event occurs, and zero otherwise. Let us assume the events can be jointly measured and the indicators return one of the following outcomes \{00, 01, 10, 11\}, where the first outcome corresponds to \(R_A\) and the second one to \(R_B\). A general probability distribution over these outcomes reads \(\mathbf{p} = \{p_{00}, p_{01}, p_{10}, p_{11}\}\). We do not assume \(A\) and \(B\)'s exclusivity and completeness, so, in general, \(p_{11} \neq 0\) and \(p_{00} \neq 0\).

Next, consider a third event \(C\) with the corresponding indicator \(R_C\). Let us first assume that all three events are jointly measurable, hence a measurement returns one of the eight outcomes \{000, 001, \ldots, 111\}, where the last position corresponds to \(R_C\). The corresponding probability distribution reads \(\mathbf{q} = \{q_{000}, q_{001}, \ldots, q_{111}\}\). If we do not make any assumptions about exclusivity and completeness, the only constraint on \(\mathbf{q}\) is

\[
q_{000} + q_{001} + \ldots + q_{111} = 1. \quad (5)
\]

Now, assume \(\mathbf{q}\) is a quasi-probability distribution, i.e., some probabilities are negative, but still sum up to one \((5)\). In order to exclude negative probabilities in the lab (we do not know what they mean), we postulate that \(A, B\) and \(C\) cannot be measured together (only \(A\) and \(B\) are co-measurable). In addition, we demand the marginal distribution over \(A\) and \(B\) to be positive:

\[
\begin{align*}
p_{00} &= q_{000} + q_{001} \geq 0, \\
p_{01} &= q_{010} + q_{011} \geq 0, \\
p_{10} &= q_{100} + q_{101} \geq 0, \\
p_{11} &= q_{110} + q_{111} \geq 0. \quad (6)
\end{align*}
\]

Remarkably, if \(q_{111} = -q_{110}\), \(A\) and \(B\) become exclusive. In addition, if \(q_{000} = -q_{001}\), we guarantee observable completeness. This shows that observable exclusivity and completeness are not fundamental but emergent.

The above quasi-probability scenario with three questions, where only two can be asked simultaneously, has been studied since the so-called Specker’s triangle discovery [6, 20]. In particular, the Specker’s triangle scenario assumes that one can measure jointly either \(A\) and \(B\), or \(A\) and \(C\), or \(B\) and \(C\). The corresponding quasi-probability distribution can be given by

\[
\begin{align*}
q^{\text{(ST)}}_{010} &= q^{\text{(ST)}}_{100} = q^{\text{(ST)}}_{110} = q^{\text{(ST)}}_{001} = q^{\text{(ST)}}_{011} = q^{\text{(ST)}}_{101} = \frac{1}{4}, \\
q^{\text{(ST)}}_{000} &= q^{\text{(ST)}}_{111} = -\frac{1}{4}. \quad (7)
\end{align*}
\]

This distribution says that whatever two questions you ask, you always find that either one or the other occurs, each with probability 1/2. For example, if one measures \(A\) and \(B\), the corresponding marginal distribution is

\[
\begin{align*}
p_{00} &= q_{000} + q_{001} = 0, \\
p_{01} &= q_{010} + q_{011} = 1/2, \\
p_{10} &= q_{100} + q_{101} = 1/2, \\
p_{11} &= q_{110} + q_{111} = 0. \quad (8)
\end{align*}
\]

Therefore, the Specker’s triangle exhibits both, the emergent exclusivity and completeness.
III. JQD CONSTRUCTION

Here we construct a JQD for an arbitrary KS set. Each KS set consists of \( N \) events, corresponding to \( \{A_1, A_2, \ldots, A_N\} \). The smallest known KS set, implementable on a quantum system, consists of \( N = 18 \) events and requires a four-dimensional Hilbert space \([27] \). There are KS subsets (called measurement contexts), corresponding to jointly measurable sets of exclusive events. Some contexts are complete subsets (recall definitions above). Each KS set consists of \( N \) events and requires a four-dimensional Hilbert space \([27] \), corresponding to jointly measurable sets of exclusive events.

Quantum realisation of a KS set consists of \( N \) rank one projectors. Each measurement context is made of mutually orthogonal projectors and each complete context \( C \) has projectors such that \( \sum_{i \in C} A_i = \mathbb{1} \). In particular, for rank one projectors, their number in the complete set equals to the Hilbert space dimension of the carrier quantum system.

We start a JQD construction with an arbitrary state preparation, assigning probability to each event from the KS set

\[
p_i \equiv p(A_i = 1) \geq 0. \tag{9}
\]

For a quantum system, we start with an arbitrary state \( \rho \) that assigns a probability \( p_i = \text{Tr}\{\rho A_i\} \) to each projector. Next, we give up the completeness assumption and allow for \( N + 1 \) outcome assignments to all the events in the KS set:

\[
\omega_i \equiv \{0, \ldots, 0 \underbrace{1}_{i-1}, 0, \ldots, 0\}, \tag{10}
\]

where \( i = 1, \ldots, N \), and

\[
\omega_0 \equiv \underbrace{0, \ldots, 0}_{N}. \tag{11}
\]

We assign to each \( \omega_i \) (\( i \neq 0 \)) the probability

\[
p(\omega_i) \equiv p_i, \quad i \neq 0. \tag{12}
\]

Finally, \( \omega_0 \) gets the following quasi-probability

\[
p(\omega_0) \equiv p_0 \equiv 1 - \sum_{i=1}^{N} p_i < 0. \tag{13}
\]

Note that \( p_0 \) is negative since for each complete measurement context \( C_c \), residing strictly in the KS set, we have

\[
\sum_{i \in C_c} p_i = 1, \tag{14}
\]

therefore

\[
1 - \sum_{i=1}^{N} p_i < 1 - \sum_{i \in C_c} p_i = 0. \tag{15}
\]

Let us show that the above construction recovers observable marginal probability distributions for all measurement contexts, including complete ones. Consider a context \( C \) related to a \( n \)-element subset \( \{A_1^{(C)}, A_2^{(C)}, \ldots, A_n^{(C)}\} \), where \( n < N \). Each \( A_i^{(C)} \) ties to a different element \( A_j \) from the KS set. The corresponding probability assignments are

\[
p_i^{(C)} = p(A_i^{(C)}), \quad i \neq 0 \tag{16}
\]

and we get

\[
\sum_{i=1}^{n} p_i^{(C)} \leq 1. \tag{17}
\]

The probability that none of the events in the context \( C \) occurs is

\[
p_0^{(C)} = (\sum_{i=0}^{N} p_i) - \left( \sum_{j=1}^{n} p_j^{(C)} \right) = 1 - \left( \sum_{j=1}^{n} p_j^{(C)} \right) \geq 0. \tag{18}
\]

Finally, if \( C \) is a complete context, i.e., \( C = C_c \), then \((14)\) holds and \( p_0^{(C_c)} = 0 \). Therefore, at the level of marginals, completeness holds.

IV. DISCUSSION

The presented JQD construction here is universal, i.e., it applies to any KS set, even a continuous measurements set. The KS theorem’s precursor, the Gleason theorem [28], deals with continuous projective measurements sets and relies on exclusivity and completeness. Thus, we can relax the Gleason’s assumptions and assign quasi-probabilities to a continuous KS set as well.

In quantum information processing and quantum computing we can think about state dependent contextuality as a resource [16, 17] carried only by certain quantum states. This picture is not as clear for SIC because any state is good, even a completely noisy one. Assigning a JQD to KS sets as discussed offers a glimpse of a solution to this problem, and perhaps, a unification of SDC and SIC. Now we can quantify how much SDC and SIC we have in a given scenario by applying known measures of JQD’s negativity [21–23]. An open problem in this context is to find an optimal JQD construction, minimizing applied negativity measure. We will tackle this in a subsequent work.

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