The existence of incompatible measurements is often believed to be a feature of quantum theory which signals its inconsistency with any classical worldview. To prove the failure of classicality in the sense of Kochen-Specker noncontextuality, one does indeed require sets of incompatible measurements. However, a more broadly applicable notion of classicality is the existence of a generalized-noncontextual ontological model. In particular, this notion can imply constraints on the representation of outcomes even within a single nonprojective measurement. We leverage this fact to demonstrate that measurement incompatibility is neither necessary nor sufficient for proofs of the failure of generalized noncontextuality. Furthermore, we show that every proof of the failure of generalized noncontextuality in a quantum prepare-measure scenario can be converted into a proof of the failure of generalized noncontextuality in a corresponding scenario with no incompatible measurements.

Measurement incompatibility—the existence of measurements that cannot be implemented simultaneously—has conventionally been taken to be part of what is truly distinctive about quantum theory relative to its classical forebears. We are here concerned with whether this attitude is justified when the notion of classicality at play is whether or not a theory (or experiment) admits of an ontological model satisfying the principle of generalized noncontextuality [1, 2]. It is already known that classical statistical theories with an epistemic restriction [3] (and subtheories of quantum theory which make the same predictions as these) can manifest incompatibility despite satisfying the principle of generalized noncontextuality. Hence, the mere fact that a theory exhibits measurement incompatibility is not sufficient to infer that it must fail to admit of a generalized-noncontextual ontological model.

In this article, we demonstrate that measurement incompatibility is also not necessary for demonstrating that quantum theory (or an experiment within quantum theory) is nonclassical in this sense. In summary, we have

\[
\text{Incompatibility } \not\overset{\text{Thm. 1}}{\Rightarrow} \text{generalized-noncontextual ontological model}
\]

Kochen-Specker notion, generalized noncontextuality has implications not only for sharp measurements but for all procedures, including unsharp measurements, preparations, and transformations. It has been found to subsume many other notions of classicality [6–10] and to shed light on the resource of nonclassicality underlying the quantum advantages known to exist for many information processing tasks [11–23].

Recall that the notion of Kochen-Specker noncontextuality is defined only for projective measurements (i.e., those whose outcomes correspond to the eigenspaces of a Hermitian operator), and the context-independence of the ontological representation of a measurement is understood as the lack of dependence on what other measurement is implemented simultaneously with it. It is well-known that the notion of Kochen-Specker noncontextuality only implies nontrivial constraints on the ontological representation if the set of measurements under consideration includes some incompatible ones.

By contrast, the notion of generalized noncontextuality provides a much broader scope of possibilities for assuming context-independence: namely, any two procedures which are operationally equivalent [1] are assumed to have the same ontological representation. As it turns out, for unsharp measurements—which in quantum theory are associated with a positive operator-valued measure (POVM) that is not projector-valued—there can be nontrivial operational equivalences between the outcomes of one and the same measurement, so that generalized noncontextuality has nontrivial implications for the ontological representation of even a single such measurement. For instance, consider the POVM \(\{\frac{1}{2}I, \frac{1}{2}1\}\) where \(I\) is the identity operator. The two outcomes of this measurement are equally likely on all states, and hence its two effects are operationally equivalent. By generalized noncontextuality, then, they must be represented in the
ontological model by the same conditional probability distribution [24].

It is the existence of such nontrivial constraints on the ontological representation of a single measurement that opens up the possibility of a proof of the failure of generalized noncontextuality without incompatibility. Note that the possibility is open only if the measurement is unsharp—any experiment involving a single projective measurement trivially admits of a generalized-noncontextual model. We demonstrate here that this possibility is in fact realized, and it is realized in the simplest operational scenario, namely, a prepare-measure experiment.

Our main result can be summarized as follows:

**Theorem 1.** From every quantum proof of the failure of generalized noncontextuality in a prepare-measure scenario involving incompatible measurements one can construct a proof that does not require any incompatibility.

In the following, the term “noncontextual” will be used as a shorthand for “generalized-noncontextual”. We will also use the expression “proof of contextuality” as a shorthand for “proof of the impossibility of a generalized-noncontextual ontological model” (even though the lesson of such proofs may well be to reject the framework of ontological models while maintaining the Leibnizian methodological principle that underlies noncontextuality [2]).

Ref. [25] makes a claim which is superficially contrary to ours, namely, that incompatibility is necessary and sufficient for proving generalized contextuality. The claim of sufficiency in Ref. [25] is only established relative to the strong assumption that the set of states under consideration includes all quantum states. This assumption is violated in any real experiment and also by many interesting subtheories of quantum theory [3, 26, 27]. The claim of the necessity of incompatibility in Ref. [25] is predicated on assuming noncontextuality for preparations alone rather than for preparations and measurements.

However, the motivation for assuming noncontextuality for preparations (namely, the Leibnizian methodological principle [2, 5]) is also a motivation for assuming it for measurements, and consequently it is unnatural to restrict the scope of the assumption to preparations alone.

Conventional no-go theorems for generalized noncontextuality— We now introduce the requisite preliminaries by describing a conventional no-go theorem for generalized noncontextuality in the usual setting of prepare-measure scenarios on a given quantum system $\mathcal{H}$. Such a scenario is depicted in Fig. 1(a). The scenario is characterized by a set of quantum states $\{\rho_s\}_s$, indexed by the preparation setting $s \in S$, and a set of POVMs, $\{\{E_{yt}\}_y\}_t$, indexed by the measurement setting $t \in T$, with elements (termed effects) in a given measurement indexed by outcomes $y \in Y$. (Note that taking the set $Y$ to be the same cardinality for all values $t \in T$ involves no loss of generality.) The observable statistics in this scenario are given by the Born rule, i.e.,

$$P^{(a)}(y|s,t) = \text{tr}(E_{yt}\rho_s).$$ (1)

The features of an operational scenario which drive any proof of contextuality are the set of operational equivalences that hold among the preparations, indexed by $a \in O_P$, and the set of operational equivalences that hold among the measurements, indexed by $b \in O_M$. These can be expressed [28] as linear constraints on the corresponding states and effects:

$$\sum_s a_s^a \rho_s = 0, \quad \sum_{y,t} \beta_{yt}^b E_{yt} = 0,$$ (2)

for all $a \in O_P$ and $b \in O_M$ where $a_s^a$ and $\beta_{yt}^b$ are real coefficients which specify the operational equivalence.

An ontological model of the prepare-measure scenario associates an ontic state space $\Lambda$ with the system $\mathcal{H}$ and explains the operational statistics as arising from stochastic processes on $\Lambda$. That is, each quantum state $\rho_s$ is represented as a probability distribution $P(\lambda|s)$ over the ontic states, $\lambda \in \Lambda$, of the system, and each measurement outcome, associated with quantum effect $E_{yt}$, is represented by a conditional probability distribution $P(y|t\lambda)$ describing the probability of outcome $y$ occurring given that the measurement was $t$ and that the ontic state was $\lambda$.

An ontological model respects the assumption of generalized noncontextuality if the ontological representations of procedures respect the operational equivalences that hold among these. For the operational equivalences of Eq. (2), generalized noncontextuality implies that

$$\sum_s a_s^a P(\lambda|s) = 0, \quad \sum_{y,t} \beta_{yt}^b P(y|t,\lambda) = 0,$$ (3)

for all $\lambda \in \Lambda$, $a \in O_P$ and $b \in O_M$.

The correlations $P(y|s, t)$ that can be realized as $P(y|s, t) = \sum_{\lambda} P(y|t, \lambda)P(\lambda|s)$ for $P(y|t, \lambda)$ and $P(\lambda|s)$ satisfying Eq. (3), i.e., those that are noncontextually realizable for the given operational equivalences, form a polytope. The facets of this polytope are examples of noncontextuality inequalities [28]. One obtains a proof of contextuality whenever the observed quantum correlations $P^{(a)}(y|s, t)$ violate at least one of these facet-defining noncontextuality inequalities. In such cases, there is no noncontextual ontological model that can reproduce the quantum correlations.

There are many known examples of such proofs [11–23, 29–34]; however, to the best of our knowledge, all previous proofs have involved a set of measurements that manifest some incompatibility.

**Measurement incompatibility**— Compatibility for generic quantum measurements—both sharp and
unsharp—is defined in terms of joint simulability [35]. For
the case of discrete outcome spaces, it can be expressed as
follows [36, 37]: the measurements associated to a set of
POVMs \{\{E_{y,t}\}_{y}\}_{t} are said to be compatible if there exists
a single measurement, described by a POVM \{G_{z}\}_{z}, and
a stochastic post-processing \(P(y|t,z)\) such that
\[
E_{y,t} = \sum_{z} P(y|t,z)G_{z}
\] (4)
for all \(y, t\). In this case, each measurement \(\{E_{y,t}\}_{y}\)
and post-processing \(P(y|t,z)\) can be simulated by first measuring \(\{G_{z}\}_{z}\)
and then implementing a post-processing of the outcome statistics
by \(P(y|t,z)\).\(^1\) If such a measurement and post-processing
do not exist, then the set of measurements is said to be
incompatible.

Note that a set consisting of a single measurement is
trivially compatible.

**Generalized noncontextuality no-go theorems without incompatibility**—We now construct a class of
operational scenarios that allow a proof of contextuality
without making use of any measurement incompatibility.

We do so by starting with a prepare-measure scenario
of the type described above—with a set of preparations
associated to states \(\{\rho_{a}\}_{a}\), a set of measurements associated to POVMs \(\{\{E_{y,t}\}_{y}\}_{t}\),
and operational equivalences described by Eq. (2)—and we implement a
modification on the measurement side. Specifically, the
modified scenario involves a single measurement which
is obtained from the set of measurements in the original
scenario by a procedure we term ‘flag-convexification’. One flag-convexifies the set of measurements by randomly
sampling a setting \(t \in T\) according to some probability
distribution \(P(t)\), then implementing the measurement
for that setting, \(\{E_{y,t}\}_{y}\), and finally outputting both \(y\) and \(t\), so that \((y, t) \in Y \times T\) constitutes the outcome of
the new effective measurement. The terminology for the
procedure stems from the fact that one is taking a convex
mixture of the measurements in the original scenario, but
one wherein the choice of measurement is not forgotten but
rather flagged, i.e., copied and fed forward to be included in
the output.

To make the argument as simple as possible, we consider uniform sampling, i.e., \(P(t) = \frac{1}{|T|}\), where \(|T|\)
is the cardinality of the set \(T\) of possible settings. (In our companion paper [4], we show that any distribution
with full support also works.) This simple version of
flag-convexification is depicted in Fig. 1. The single
measurement in the flag-convexified scenario is associated
to a POVM \(\{E_{y,t}\}_{y,t}\) defined by
\[
\tilde{E}_{y,t} := \frac{1}{|T|} E_{y,t}.
\] (5)
It is straightforward to check that this is a valid
POVM. For ease of bookkeeping, effects and conditional probability distributions which refer to the
flag-convexified scenario will be denoted with a tilde.

![FIG. 1. (a) The original prepare-measure scenario. (b) The flag-convexified scenario, where the white dot represents the
copying of \(T\).](image)

Note that the correlations in the original scenario
are naturally associated with a conditional probability
distribution of the form \(P^{(a)}(y|s, t) := \text{tr}(E_{y|t}\rho_{s})\) where \(t\) is on the right-hand-side of the conditional, while the
correlations in the flag-convexified scenario are naturally
associated with a conditional probability distribution of the form \(\tilde{P}^{(a)}(y, t|s) := \text{tr}(\tilde{E}_{y,t}\rho_{s})\) where \(t\) is on the
left-hand-side of the conditional. Using Eq. (5) and the
linearity of the Born rule, these are related simply by
\[
\tilde{P}^{(a)}(y, t|s) = \frac{1}{|T|} P^{(a)}(y|s, t).
\] (6)

Since the set of preparations in the flag-convexified
scenario is identical to the set in the original scenario,
it follows that the operational equivalences for the
preparations are unchanged relative to Eq. (2),
\[
\sum_{s} \alpha_{s}^{(a)} \rho_{s} = 0,
\] (7)
for all \(a \in O_{P}\). Consider now the operational equivalences
among the effects in the new scenario. Substituting Eq. (5)
into Eq. (2), one finds that the operational equivalences in the
flag-convexified scenario are given by
\[
\sum_{y, t} \beta_{y,t}^{(b)} \tilde{E}_{y,t} = 0
\] (8)
for all \(b \in O_{M}\). So the effects \(\tilde{E}_{y,t}\) in the flag-convexified
scenario satisfy linear constraints of exactly the same form
as those satisfied by the effects \(E_{y,t}\) from the original
scenario.

\(^1\) An equivalent definition of compatibility can be obtained by
replacing stochastic post-processing by coarse-graining (see, e.g.,
Lemma 1 of Ref. [37]). For sharp measurements, it is well known
that this definition of compatibility reduces to commutation of
the associated Hermitian operators (see Proposition 8 of Ref. [38]
and Theorem 1 of Ref. [39] for proofs of some generalizations of this
result).
An ontological representation of the flag-convexified scenario represents each state $\rho_s$ by some probability distribution $\tilde{P}(\lambda|s)$ and each effect $E_{y,t}$ by some conditional probability distribution $\tilde{P}(y,t|\lambda)$. Given the operational equivalences of Eqs. (7) and (8), the assumption of noncontextuality implies that $\tilde{P}(\lambda|s)$ and $\tilde{P}(y,t|\lambda)$ must satisfy

$$\sum_s \alpha_s^{(a)} \tilde{P}(\lambda|s) = 0, \quad \sum_{y,t} \beta_{y,t}^{(b)} \tilde{P}(y,t|\lambda) = 0,$$

for all $\lambda \in \Lambda$, $a \in O_P$ and $b \in O_M$, which are seen to be of the same form as Eq. (3).

In the appendix, we prove that there exists a noncontextual ontological model for the original scenario if and only if there exists a noncontextual ontological model for the flag-convexified scenario. This fact implies that every no-go theorem for noncontextuality in a prepare-measure scenario involving incompatibility (of which there are many) can be transformed via flag-convexification into a no-go theorem in a scenario that involves only a single measurement (and hence involves no incompatibility). This establishes Theorem 1.

An example not built from processings of incompatible sharp measurements— The opportunity for proving generalized contextuality without incompatibility arises from the fact that there can be nontrivial operational equivalences between the outcomes of one and the same measurement if the latter is unsharp. It is natural to ask whether this opportunity only presents itself when the unsharp measurement is a flag-convexification (or stochastic post-processing) of a set of incompatible sharp measurements and when the operational equivalences in the former are implied by the conventional variety of operational equivalences in the latter. If it did, then one might dismiss proofs without incompatibility as simply proofs with incompatibility “in disguise”. As we now demonstrate, the question is answered in the negative—there are genuinely novel types of proofs of contextuality for unsharp measurements.

Consider a prepare-measure scenario with five preparations, associated with the set of normalized rank-1 projectors $\{\rho_s = |\psi_s\rangle \langle \psi_s|\}^5_{s=0}$ where

$$|\psi_s\rangle := \cos\left(\frac{\pi}{5}s\right)|0\rangle + \sin\left(\frac{\pi}{5}s\right)|1\rangle$$

and a single 5-outcome measurement, associated with the POVM $\{E_{y}\}^5_{y=0}$ where the effects are defined as $E_y = \frac{1}{5}\rho_y$ (i.e., subnormalized versions of the projectors onto the states) and thus sum to the identity.

These quantum states and effects can be represented as real-valued vectors in the space of Hermitian operators using the basis of Pauli operators. Because they all have zero component of the $Y$ Pauli, they can be represented in the three-dimensional space spanned by $I$, $Z$, and $X$ Paulis. We provide these representations in Figs. 2(a) and (b) respectively. For five vectors in a three-dimensional space, there are necessarily linear dependences amongst them, which can be captured by a pair of equations. For the five states, these are interpreted as a pair of operational equivalences. They can be expressed as:

$$\rho_0 - q\rho_1 + q\rho_2 - \rho_3 = 0,$$

$$\rho_1 - q^2\rho_2 + q\rho_4 = 0,$$

where $q$ is the golden ratio, namely $q = 2\cos(\pi/5) = (1 + \sqrt{5})/2$. The five effects satisfy the same operational equivalence relations (substituting $E_i$ for $\rho_i$ in Eq. (11)) because they are equal to the states up to a normalization factor.

By applying the linear programming techniques of Ref. [40] to this scenario, we can compute facet-defining noncontextuality inequalities. (Further details are provided in the appendix.)

Consider a conditional probability distribution $P(y|s)$ (whose elements we will abbreviate as $p_{y|s}$) and the following linear combination of these elements:

$$C := q(p_{1|10} + p_{1|12}) + (q - 1)p_{2|10} + p_{0|2} - (q + 1)p_{1|1}.$$

An inequality that defines a facet of the polytope of noncontextually realizable conditionals $P(y|s)$ is found to be:

$$C \geq 0.$$

Meanwhile, the quantumly realizable correlations for the scenario described above yield

$$C^{(q)} = \frac{q^2 - 4}{10} \approx -0.138,$$

which violates the noncontextuality inequality of Eq. (13), thereby proving that the quantum scenario does not admit of a noncontextual model.
Finally, we demonstrate that the 5-outcome POVM used in this proof cannot be understood as the flag-convexification of a set of projector-valued measures (PVMs), nor even as a stochastic processing of a set of PVMs. (Recall that sharp measurements in quantum theory are represented by PVMs.) Suppose that the 5-outcome POVM \( \{E_0, \ldots, E_4\} \) could be obtained by stochastic processing of a set \( \{P^{(\alpha)}\}\) of distinct binary-outcome qubit PVMs, \( P^{(\alpha)} := \{\Pi^{(\alpha)}_0, \Pi^{(\alpha)}_1\} \). Specifically, this would mean that 
\[
E_y = \sum_{j,k} P(y|j,k) \left( \sum_{\alpha} \Pi^{(\alpha)}_j P(\alpha,k) \right)
\]
for some auxiliary variable \( k \), distribution \( P(\alpha,k) \) and conditional \( P(y|j,k) \). However, because each effect \( E_y \) is itself rank-1 and because all the \( \Pi^{(\alpha)} \) are distinct, these sums (which are non-negative by virtue of the weights \( P(y|j,k) P(\alpha,k) \) being non-negative) can each contain only a single rank-1 projector. Moreover, because post-selection is not allowed in such a processing, each projector must appear in the positive sum yielding some effect. It follows that there must be a one-to-one association between the five effects and the full set of projectors. But this yields a contradiction. One way to see this is that no two effects are orthogonal, while the complementary rank-1 projectors appearing in a single PVM, \( \Pi^{(\alpha)}_0 \) and \( \Pi^{(\alpha)}_1 \), are orthogonal. (Alternatively, one can note simply that there are an odd number of effects in the POVM and an even number of projectors in the set of PVMs.)

**Related work**— Ref. [41] has also noted that there is an opportunity for leveraging operational equivalences among the elements of a single unsharp measurement in proofs of generalized contextuality\(^2\)—indeed, the construction they consider is an instance of what we here termed flag-convexification. The analysis in Ref. [41], however, makes use of an auxiliary assumption, namely, that the probability distribution over ontic states after a measurement is proportional to the response function of the effect that was observed. This assumption was not shown to follow from noncontextuality, so Ref. [41] does not establish our result.\(^3\)

It is also worth drawing the parallel between our work and that of Fritz [42, 43], which established that there are Bell-like causal compatibility inequalities [42, 44–46] admitting of quantum violations even in scenarios where each party implements only a single measurement, implying that incompatibility is also not necessary for exhibiting quantumness in such cases.

**Conclusions**— We have demonstrated that incompatibility is not required for proofs of generalized contextuality. This fact shows a new sense in which the failure of generalized noncontextuality can be proven in a broader range of scenarios than the failure of Kochen-Specker noncontextuality. This result also opens the door to the possibility of finding new quantum advantages for information processing by considering operational scenarios with no incompatibility, some of which might have previously been overlooked by virtue of mistakenly being thought to offer no opportunity for nonclassical phenomena.

Our companion paper, Ref. [4], generalizes the results in this paper in a number of ways. First, the arguments therein are formulated in the context of arbitrary generalized probabilistic theories rather than just quantum theory. This means that if a given generalized probabilistic theory admits of a proof of contextuality in a prepare-measure scenario, then one can find such a proof involving only a single measurement. Second, we demonstrate the possibility of proofs of contextuality (for both quantum theory and GPTs) in scenarios that have only a single preparation device as well as a single measurement device. Such scenarios have no external inputs at all. Hence, in addition to not requiring any incompatibility, they also do not require the freedom of choice assumption—roughly, that one can choose one’s external inputs freely. Finally, we show that if one’s detectors are inefficient, in that they have probability \( p \) of performing ideally and probability \( 1-p \) of failing to give any outcome, then one can still witness contextuality, even for arbitrary inefficiencies, i.e., any \( p > 0 \). That is, there is no detector loophole for tests of generalised noncontextuality.

**Acknowledgements.**— This research was supported by Perimeter Institute for Theoretical Physics. Research at Perimeter Institute is supported by the Government of Canada through the Department of Innovation, Science and Economic Development Canada and by the Province of Ontario through the Ministry of Research, Innovation and Science. DS, and ABS acknowledge support by the Foundation for Polish Science (IRAP project, ICTQT, contract no.2018/MAB/5, co-financed by EU within Smart Growth Operational Programme). JHS was supported by the National Science Centre, Poland (Opus project, Categorical Foundations of the Non-Classicality of Nature, project no. 2021/41/B/ST2/03149). RK is supported by the Chargé de Recherche fellowship of the Fonds de la Recherche Scientifique - FNRS (F.R.S.-FNRS), Belgium. All of the diagrams within this manuscript were prepared using TikZit. Figures were prepared using Tikz.

\(^2\) In fact, Ref. [41] claims that the notion of noncontextuality proposed in Ref. [1] must be supplemented with an additional constraint: that if two effects \( E \) and \( E' \) satisfy \( E' = sE \) where \( s \in [0,1] \), then the conditional probability distributions that represent them, \( P(E|\lambda) \) and \( P(E'|\lambda) \), must satisfy \( P(E'|\lambda) = sP(E|\lambda) \). However, this constraint is not an innovation to the notion of noncontextuality, but rather is known to follow from the representation of post-processing within any ontological model, as noted in Ref. [24] (see the proof of condition NC3 therein).

\(^3\) Additionally, we were not able to show that this assumption follows from noncontextuality. Furthermore, if one reconsiders their scenario as a prepare-measure experiment, so that one can apply the techniques of Ref. [28], we do not obtain the inequalities from Ref. [41] as valid noncontextuality inequalities.
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It then straightforwardly follows that every no-go theorem for noncontextuality in a prepare-measure scenario involving incompatibility can be transformed (via flag-convexification) into a no-go theorem involving a single measurement, that is, into a no-go theorem without incompatibility.

We begin with the forward implication. It suffices to take

\[ \tilde{P}(\lambda|s) := P(\lambda|s), \quad \tilde{P}(y,t|\lambda) := \frac{1}{|T|} P(y|t,\lambda). \]  

(17)

It is straightforward to check that \( \tilde{P}(y,t|\lambda) \) is a valid conditional probability distribution. From the fact that \( P(\lambda|s) \) and \( P(y|t,\lambda) \) satisfy the noncontextuality constraints in Eq. (3) from the main text, it follows immediately that \( \tilde{P}(\lambda|s) \) and \( \tilde{P}(y,t|\lambda) \) satisfy the noncontextuality constraints in Eq. (9) from the main text. Eq. (16) then follows from Eq. (15) by making use of Eqs. (6) from the main text and (17), i.e.,

\[ \tilde{P}^{(n)}(y,t|s) = \frac{1}{|T|} \sum_{\lambda} P^{(n)}(y|t,\lambda) P(\lambda|s) \]  

(18)

\[ = \frac{1}{|T|} \sum_{\lambda} \tilde{P}(y,t|\lambda) \tilde{P}(\lambda|s). \]  

(19)

\[ = \tilde{P}(y,t|\lambda). \]  

(20)

The reverse implication follows by an analogous argument, but where one defines \( P(\lambda|s) := \tilde{P}(\lambda|s) \) and \( P(y|t,\lambda) := |T| \tilde{P}(y,t|\lambda) \).

**Proof of noncontextuality inequality**

We seek to put bounds on the correlations in the prepare-measure experiment. These are given in the text in terms of \( P(y|s) \), where \( y \) runs over the five outcomes of the measurement and \( s \) runs over the five preparations. In an ontological model, we have

\[ P(y|s) = \sum_{\lambda} P(y|\lambda) P(\lambda|s). \]  

(21)

But by implementing a Bayesian inversion between \( \lambda \) and \( s \), this can also be expressed as

\[ P(y|s) = \sum_{\lambda} \tilde{P}(y|\lambda) P(s|\lambda) P(\lambda) P(s)^{-1}. \]  

(22)

We here assume a uniform prior over \( s \), i.e., \( P(s) = 1/5 \). In this case, whatever linear dependences hold among the \( P(\lambda|s) \) for a given \( \lambda \), the same linear dependences hold among the \( P(s|\lambda) \) for a given \( \lambda \). It will be convenient below to focus on the joint distribution \( P(y,s) \), which takes the form

\[ P(y,s) = \sum_{\lambda} P(y|\lambda) P(s|\lambda) P(\lambda). \]  

(23)
For a uniform prior, this is related to $P(y|s)$ by a constant factor.

We now derive the constraints on $P(y,s)$ that are implied by the assumption of noncontextuality and the operational equivalences that hold among the states and among the effects.

Recall that the assumption of noncontextuality means that operational equivalences of the form of Eq. (2) in the main text imply corresponding constraints on the representations of states and effects in the ontological model, namely, Eqs. (3) from the main text.

The particular form of operational equivalences appearing in the pentagon example are

$$
\rho_0 - q\rho_1 + q\rho_2 - \rho_3 = 0, \\
\rho_1 - q\rho_2 + q\rho_3 - \rho_4 = 0,
$$

(24)

where $q = 2\cos(\pi/5) = (1 + q)/2$ (the golden ratio), and

$$
E_0 - qE_1 + qE_2 - E_3 = 0, \\
E_1 - qE_2 + qE_3 - E_4 = 0.
$$

(25)

Given the five-fold symmetry of the set of states, the linear dependence relations described by the pair of equations in Eq. (24) can be equivalently expressed by the image of this pair of equations under any cyclic permutation of the five states. Similarly, the five-fold symmetry of the set of effects implies that the linear dependence relations described by the pair of equations in Eq. (25) are equivalent to those obtained by cyclic permutations of the effects.

Note that there is an intuitive justification of the operational equivalence in the first equation of Eq. (24): the ensemble consisting of pure states $\rho_0$ and $\rho_2$, drawn with probabilities $1/(q + 1)$ and $q/(q + 1)$ respectively, yields the same density operator as the ensemble consisting of pure states $\rho_1$ and $\rho_3$, drawn with probabilities $q/(q + 1)$ and $1/(q + 1)$, respectively:

$$
\frac{1}{q + 1}\rho_0 + \frac{q}{q + 1}\rho_2 = \frac{q}{q + 1}\rho_1 + \frac{1}{q + 1}\rho_3.
$$

(26)

This equality is easily verified by considering the geometry of the five states in the Bloch sphere (Fig. 3). The weight of $\rho_0$ in the mixed state $\rho$ (indicated in Fig. 3) is proportional to the Euclidean distance between $\rho$ and $\rho_2$, while the weight of $\rho_2$ is proportional to the Euclidean distance between $\rho$ and $\rho_0$. The ratio of these two Euclidean distances is $1/q$ where $q$ is the golden ratio, since this is one of the ways in which the golden ratio appears in the geometry of the pentagon. It follows that the ratio of the weight of $\rho_0$ to the weight of $\rho_2$ in the mixed state $\rho$ is also $1/q$. Requiring that these weights sum to unity then implies that they must be $1/(q + 1)$ and $q/(q + 1)$ respectively. The fact that $\rho_3$ and $\rho_1$ respectively have the same Euclidean distances to $\rho$ as do $\rho_0$ and $\rho_2$ implies that $\rho_3$ and $\rho_1$ also appear with weights $1/(q + 1)$ and $q/(q + 1)$ in a convex decomposition of $\rho$. Equating the two convex decompositions of $\rho$ yields Eq. (26).

The second operational equivalence relation in Eq. (24) is justified similarly, and the symmetry of these relations under cyclic permutations of the states is also evident from the geometry. A similar analysis holds for the operational equivalence relations in Eq. (25).

Generalized noncontextuality is the assumption that for each operational equivalence among states or among effects, one must posit a corresponding constraint on the ontological representation of these states and effects. Thus, in the concrete example considered here, for each $\lambda$, the $P(|s|s)$ satisfy linear dependency conditions parallel to those of Eq. (24). Furthermore, as noted above, for each $\lambda$, the Bayesian inverses of these conditionals, $P(s|\lambda)$, must satisfy the same linear dependence conditions as the $P(|s|s)$, together with normalization. Consequently, we have the constraints:

$$
P(s = 0|\lambda) - qP(s = 1|\lambda) + qP(s = 2|\lambda) - P(s = 3|\lambda) = 0, \\
P(s = 1|\lambda) - qP(s = 2|\lambda) + qP(s = 3|\lambda) - P(s = 4|\lambda) = 0, \\
\sum_s P(s|\lambda) = 1.
$$

(27)

For the effects, generalized noncontextuality implies that the $P(y|\lambda)$ must satisfy linear dependence conditions parallel to those of Eq. (25), together with normalization, so that

$$
P(y = 0|\lambda) - qP(y = 1|\lambda) + qP(y = 2|\lambda) - P(y = 3|\lambda) = 0, \\
P(y = 1|\lambda) - qP(y = 2|\lambda) + qP(y = 3|\lambda) - P(y = 4|\lambda) = 0, \\
\sum_y P(y|\lambda) = 1.
$$

(28)

The constraints in Eq. (27) must hold for every ontic state $\lambda$. If a probability distribution on $s$, i.e., $(P(s = 0), P(s = 1), P(s = 2), P(s = 3), P(s = 4))$, satisfies these constraints, then it is termed a noncontextual assignment to $s$. In a noncontextual model, every ontic state $\lambda$...
makes such an assignment, which describes what one can retrodict about $s$ given $\lambda$.

Similarly, if a probability distribution on $y$, i.e., $(P(y = 0), P(y = 1), P(y = 2), P(y = 3), P(y = 4))$, satisfies the constraints in Eq. (28), then it is termed a noncontextual assignment to $y$. Again, every ontic state $\lambda$ makes such an assignment in a noncontextual model, describing what one can predict about $y$ given $\lambda$.

It is useful to consider the set of all possible noncontextual assignments to $s$. By the linearity of the constraints, any convex mixture of a pair of noncontextual assignments is also a valid noncontextual assignment, so the set is convex. In fact, it is a polytope contained within the 5-vertex simplex of all probability assignments over $s$.

Given that the possible noncontextual assignments to $y$ satisfy precisely the same constraints as the noncontextual assignments to $s$ (since Eqs. (27) and (28) have the same form), these describe precisely the same polytope. We turn now to the description of this polytope.

Because of the invariance of the constraints under a cyclic permutation of the five components of the probability distribution, it follows that any cyclic permutation of the components of a noncontextual assignment yields a noncontextual assignment.

In fact, there are precisely five vertices of the polytope of noncontextual assignments, namely, the cyclic permutations of the following assignment:

\[
\frac{1}{\sqrt{5}} (1, q^{-1}, 0, 0, q^{-1}).
\] (29)

One can easily verify that this probability distribution satisfies Eq. (27) (or Eq. (28)) and satisfies normalization (it suffices to recall that the golden ratio $q$ satisfies $q^{-1} = q - 1$ and $1 + 2q^{-1} = \sqrt{5}$). Extremality can be verified by mathematical software.\(^4\)

Let $\kappa$ vary over the five extremal noncontextual assignments to $y$ and let $\kappa'$ vary over the five extremal noncontextual assignments to $s$. For every ontic state $\lambda$, the noncontextual assignment to $y$ must be a convex mixture of the extremal ones: $P(y|\lambda) = \sum_\kappa P(y|\kappa)P(\kappa|\lambda)$ for some $P(\kappa|\lambda)$. Similarly, the noncontextual assignment to $s$ by any ontic state $\lambda$ must be a convex mixture of the extremal ones: $P(s|\lambda) = \sum_{\kappa'} P(s|\kappa')P(\kappa'|\lambda)$ for some $P(\kappa'|\lambda)$. It follows that Eq. (23) can be rewritten as:

\[
P(y,s) = \sum_{\kappa,\kappa'} P(y|\kappa)P(s|\kappa')P(\kappa,\kappa').
\] (30)

where $P(\kappa,\kappa') = \sum_\lambda P(\kappa|\lambda)P(\kappa'|\lambda)P(\lambda)$ describes an arbitrary distribution over $\kappa$ and $\kappa'$, and where the

\(4\) The presence of irrational coefficients complicates the task of identifying the extremal solutions to a set of linear constraints. For very small problems, such as the one here, however, it can be tackled by Mathematica\(^\circ\).

\(5\) It should be noted that we have conceptualized the prepare side

PROOF OF NONCONTEXTUALITY INEQUALITY

We denote this twenty-five-ray unbounded hypercone by $T_{\text{unbounded}}$. The intersection of $T_{\text{unbounded}}$ with the hyperplane defining the uniform marginal condition (i.e., the hyperplane where $\sum_y P(y, s) = 1/5$ for all $s$) defines a bounded polytope which we will denote by $T_{\text{bounded}}$. $T_{\text{bounded}}$ is the polytope of noncontextually realizable joint distributions $P(y, s)$ with uniform marginal on $s$, for the given operational equivalences. One could seek to identify the vertices and facet inequalities of $T_{\text{bounded}}$, but this is computationally nontrivial and it is not necessary for witnessing the failure of noncontextuality. For any distribution $P(y, s)$ with uniform marginal on $s$, violation of any facet inequality of the hypercone $T_{\text{unbounded}}$ is sufficient to witness the fact that this distribution does not lie within $T_{\text{bounded}}$. Therefore, we here make use of some of the facet inequalities of $T_{\text{unbounded}}$ as our noncontextuality inequalities.

The polytope of noncontextually realizable conditional distributions $P(y|s)$, denoted $T_{\text{bounded}}^c$, is simply the image of $T_{\text{bounded}}$ under the map that rescales every joint distribution $P(y, s)$ with uniform marginal on $s$ by the factor 5, since for such distributions $P(y|s) = P(y, s)/P(s) = 5P(y, s)$. That is, $T_{\text{bounded}}^c$ is the intersection of $T_{\text{unbounded}}$ with the hyperplane where $\sum_y P(y|s) = 1$ for all $s$. Since the hypercone $T_{\text{unbounded}}$ is invariant under nonnegative rescaling, we find that its facet inequalities constitute both noncontextuality inequalities for conditional distributions $P(y|s)$ or for joint distributions $P(y, s)$ with uniform marginals.\(^5\)

To identify facet inequalities of the hypercone $T_{\text{unbounded}}$ from its extremal rays, one can use linear
programming algorithms. Each facet inequality yields a noncontextuality inequality for this scenario. By applying standard such algorithms, we find that one such facet inequality is $C \geq 0$, where, using the shorthand notation $p(y|s) := P(y|s)$, we can write $C$ as

$$C := q(p_{1|0} + p_{1|2}) + (q-1)p_{2|0} + p_{0|2} - (q+1)p_{1|1}. \quad (32)$$

Consequently, if a conditional distribution $P(y|s)$ violates the inequality $C \geq 0$, the possibility of a noncontextual model for the given operational equivalences is ruled out. One can easily verify that the extremal assignments (i.e., permutations of the rows and columns of Eq. (31)) satisfy this inequality.

Note that since the hypercone $T_{\text{unbounded}}$ is invariant under uniform rescaling, by substituting $p(y|s) \rightarrow 5p(y|s) := P(y,s)$ we obtain the equally valid inequality $C' \geq 0$, where

$$C' := q(p_{1,0} + p_{1,2}) + (q-1)p_{2,0} + p_{0,2} - (q+1)p_{1,1} \quad (33)$$

which is satisfied by all $P(y,s)$ with uniform marginal $P(s)$ which admit a noncontextual model for the same operational equivalences.

One can generate forty-nine more facet inequalities of $T_{\text{unbounded}}$ by leveraging some of the symmetries of the problem. Since the set of extremal rays of $T_{\text{unbounded}}$ remains closed under the replacing $p(y|s)$ with $p_{\pi(y)|\pi'(s)}$ where $\pi$ and $\pi'$ are cyclic permutations, or by replacing $p(y|s)$ with $p_{\pi(s)}$, it follows that any inequality generated by applying the inverse of such replacement to Eq. (12) from the main text would also constitute a facet-defining inequality of $T_{\text{unbounded}}$.

For the prepare-measure scenario described in the main text and depicted in Fig. (2) in the main text, the quantum realized data set has elements $p(y|s) = \text{Tr}(\rho_{s}E_{y})$. Computing these overlaps, the conditional distribution is described by the following $5 \times 5$ matrix:

$$M^{(q)} := \frac{1}{10} \begin{pmatrix} 4 & 1+q & 2-q & 2-q & 1+q \\ 1+q & 4 & 2-q & 2-q & 1+q \\ 2-q & 4 & 1+q & 2-q & 1+q \\ 2-q & 4 & 1+q & 2-q & 1+q \\ 1+q & 2-q & 2-q & 1+q & 4 \end{pmatrix}. \quad (34)$$

One easily verifies that if one evaluates $C$ in Eq. (12) from the main text for $M^{(q)}$, one obtains the value $\frac{q^{2}-4}{10} \approx -0.138$ reported in Eq. (14) of the main text, which is a violation of the noncontextuality inequality in Eq. (13) from the main text.