Representing probabilistic data via ontological models

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Ontological models are attempts to quantitatively describe the results of a probabilistic theory, such as Quantum Mechanics, in a framework exhibiting an explicit realism-based underpinning. Unlike either the well known quasi-probability representations, or the “r-p” vector formalism, these models are contextual and by definition only involve positive probability distributions (and indicator functions). In this article we study how the ontological model formalism can be used to describe arbitrary statistics of a system subjected to a finite set of preparations and measurements. We present three models which can describe any such empirical data and then discuss how to turn an indeterministic model into a deterministic one. This raises the issue of how such models manifest contextuality, and we provide an explicit example to demonstrate this.

In the second half of the paper we consider the issue of finding ontological models with as few ontic states as possible.

I. INTRODUCTION

Entanglement plays an important role in both quantum foundations and quantum information. Recently however, an overlap between these two fields has emerged which goes beyond this somewhat obvious reason for common interest. For instance, there is mounting evidence that contextuality plays a role in any enhancement of quantum over classical communication protocols [1]. A second example is work on the “r-p” framework for analyzing the information processing power of general (not necessarily quantum) probabilistic theories [2, 3, 4, 5] - a body of work to which this paper is closely related. Finally we mention work by one of us [6] showing that one particular class of ontological models [7, 8] (or ‘hidden variable theories’) of quantum mechanics has a computational power slightly greater than that of regular quantum computation (if access to values of the hidden variables is granted).

As in this last example, we will be considering ontological models. Such models reproduce the predictions of quantum mechanics by using (positive, normalized) probability distributions over a space of (sometimes, though not always, hidden) variables to describe the state of a system. Unlike quantum states in operational quantum mechanics, these variables are presumed to correspond directly to “properties of reality” in some fashion - hence we term the variables the ontic states. Measurements in these models are described by positive valued indicator functions - functions which simply determine the probability of a system in a given ontic state yielding the particular measurement outcome associated with that indicator function. In this way ontological models differ from the many well known quasi-probability representations of quantum mechanics. In those representations, even if the states are represented by positive, normalized probability distributions (e.g. the Q-function), the measurements will be represented by indicator functions which can be negative (or greater than 1). Such negativity is difficult to interpret if one is interested in describing properties of a reality underpinning quantum mechanics. In fact Spekkens has shown that such negativity arises in these representations precisely because they are assumed non-contextual [9]. In particular, this assumption of non-contextuality is made in the work on the r-p formalism mentioned above, and is the reason the r-vectors (those vectors associated with measurements) generally have to contain negative elements. Similar considerations apply to the work on discrete Wigner distributions [10].

A comprehensive discussion of the ontological model framework was undertaken in [7]. For our purposes we will not need the majority of the formalism developed in that paper. However, let us mention in passing a few of the conclusions from it. Firstly, there exist a wide variety of ontological models, both deterministic and indeterministic, including ones which, unlike the examples given in [6], do not provide greater computational power than that of regular quantum computation. Secondly, for some models it is necessary to consider not just ontic states of the system under consideration, but also those of the preparation and measurement devices. Thirdly, the manner in which such models exhibit contextuality is varied, but one feature (which in some sense subsumes contextuality) that is common to all models is a property we term deficiency. Loosely speaking, deficiency breaks a symmetry between preparations and measurements in quantum mechanics. It is the property that the set of ontic states which a system prepared in quantum state $|\psi\rangle$ may actually be in, is strictly smaller than the set of ontic states which would reveal the measurement outcome $|\psi\rangle\langle\psi|$ with certainty.

In this paper, we initiate an investigation into how ontological models can be used to reproduce quantum mechanical statistical predictions for a discrete set of preparations of, and measurements upon, a given system. We start in section II by discussing a method of representing
empirical data in matrix form. In Section III we then introduce a matrix factorization of this data, equivalent to an ontological model over a finite number of ontic states. In Sections III B, III C and III D we present three factorizations which can describe any such empirical data. We then discuss in section III E how to turn an indeterministic ontological model into a deterministic one. This raises the issue of how such models manifest the necessary contextuality, and in Section III F we discuss this and provide an explicit example.

In the second half of the paper, Section IV, we consider the issue of finding ontological models with as few ontic states as possible—a topic with potential application to the classical simulation of quantum systems.

II. DATA TABLES

We begin with a common [2, 3, 4, 5], although somewhat idealistic, formalization of the process of performing an experiment resulting in probabilistic data—data for which we then seek an explanation. The experiment consists of a set of preparation procedures, and a set of measurement procedures [26]. The preparation procedures are defined in terms of different macroscopic (and therefore distinguishable) configurations (settings) of an apparatus, and these are labeled \( P^{(i)} \), where \( i = 1, 2, \ldots, s \) (\( s \) standing for "states"). Likewise the different measurement procedures are macroscopically distinguishable, and can be labeled \( M^{(i)} \), where \( i = 1, 2, \ldots, m \). Each measurement procedure has some number \( d \) of outcomes, which, by padding with null outcomes if necessary, we take to be the same for each. We can then label the occurrence of the \( k \)th outcome, when the measurement procedure is \( M^{(i)} \), as \( M^{(i)}_{k} \).

We imagine that a large number of experiments are performed, and the probabilities that a given preparation yields a given measurement outcome estimated and tabulated, e.g.

\[
\begin{align*}
P^{(1)} & \quad P^{(2)} & \quad P^{(3)} & \quad P^{(4)} \\
M^{(1)}_{1} & 0.08 & 0.21 & \ldots & \ldots \\
M^{(1)}_{2} & 0.51 & 0.63 & \ldots & \ldots \\
M^{(1)}_{3} & 0.41 & 0.16 & \ldots & \ldots \\
M^{(2)}_{1} & 0.35 & 0.72 & \ldots & \ldots \\
M^{(2)}_{2} & 0.60 & 0.21 & \ldots & \ldots \\
M^{(2)}_{3} & 0.05 & 0.06 & \ldots & \ldots \\
\end{align*}
\]

In this example \( s = 4, m = 2 \) and \( d = 3 \), so that there are \( dm \) rows in the matrix. The sum of every \( d \) elements within each column must be 1, since one of the outcomes must obtain for every measurement. For clarity we have drawn a horizontal line underscoring the separation between distinct measurements.

We will call such a matrix of values a data table, and generally denote it \( D \). It will often be convenient to consider \( D \) a three-dimensional array, where the particular measurement being performed lies along the third dimension. For the above example we can do so by defining

\[
D^{(1)} = \begin{pmatrix}
P^{(1)} & P^{(2)} & P^{(3)} & P^{(4)} \\
M^{(1)}_{1} & 0.08 & 0.21 & \ldots & \ldots \\
M^{(1)}_{2} & 0.51 & 0.63 & \ldots & \ldots \\
M^{(1)}_{3} & 0.41 & 0.16 & \ldots & \ldots \\
M^{(2)}_{1} & 0.35 & 0.72 & \ldots & \ldots \\
M^{(2)}_{2} & 0.60 & 0.21 & \ldots & \ldots \\
M^{(2)}_{3} & 0.05 & 0.06 & \ldots & \ldots \\
\end{pmatrix}
\]

More generally the data table can be taken as specified in terms of \( D^{(x)}_{i,j} \), where \( x = 1, 2, \ldots, m \), \( i = 1, 2, \ldots, d \), \( j = 1, 2, \ldots, s \).

Now in quantum mechanics we generally associate a density matrix \( \rho_{k} \) with a preparation \( P^{(k)} \), and a POVM element \( E^{(x)}_{i} \) with a measurement outcome \( M^{(x)}_{i} \). Since we will frequently be considering data tables for which the table entries are presumed to be given by quantum mechanical expectations—i.e. \( \text{Tr}(\rho_{k} E^{(x)}_{i}) \)—it is often convenient to label the rows and columns via the appropriate quantum operators. In fact, we will almost always only be considering procedures which correspond to pure quantum states \( \psi_{k} \) and to sets of sharp (projective) measurements \( \{\Pi_{i}\} \) (also known as PVM’s). In this case we have

\[
D^{(x)}_{i,k} = \langle \psi_{k} | \Pi^{(x)}_{i} | \psi_{k} \rangle,
\]

and it will be convenient to adopt a more quantum notation along the lines of:

\[
\begin{pmatrix}
\psi_{1} & \psi_{2} & \psi_{3} & \psi_{4} \\
\Pi^{(1)} & 0.08 & 0.21 & \ldots & \ldots \\
\Pi^{(2)} & 0.51 & 0.63 & \ldots & \ldots \\
\Pi^{(3)} & 0.41 & 0.16 & \ldots & \ldots \\
\Pi^{(4)} & 0.35 & 0.72 & \ldots & \ldots \\
\Pi^{(5)} & 0.60 & 0.21 & \ldots & \ldots \\
\Pi^{(6)} & 0.05 & 0.06 & \ldots & \ldots \\
\end{pmatrix}
\]

At this stage it is pertinent to consider the following:

**Proposition 1** Every possible data table can be realized via standard quantum expectation values of projective measurements on pure states.

At first sight this proposition may appear incorrect. Consider, for example, the following data table:

\[
\begin{pmatrix}
\psi_{1} & \psi_{2} \\
\Pi^{(1)} & 1 & 0 \\
\Pi^{(2)} & 0 & 1 \\
\Pi^{(3)} & 1/2 \\
\Pi^{(4)} & 0 & 1/2 \\
\end{pmatrix}
\]
As there are two possible outcomes for each measurement, one might surmise that the data was generated by sharp measurements on a qubit prepared in either $|\psi_1\rangle$ or $|\psi_2\rangle$. In that case the table is clearly impossible - the first measurement implies the two states are orthogonal, and the second implies there is a two outcome measurement which yields one of the states with certainty, but which is unbiased with respect to the second state. However, consider if the system was quantum mechanically actually a three dimensional qutrit with basis states $(0), (1), (2)$. In this case it is easy to verify that choosing $|\psi_1\rangle = (0), |\psi_2\rangle = (1)$, the two sets of measurements could be $\{00, 22\}, 11\}$ and $\{00, 0+, 1+, 1-\}$. That is, the states are sharp and the measurements are projective. The point is that there is no way of determining from the raw data table itself any presumed (quantum) Hilbert space dimension of the systems under investigation. We will use the general notation $d_Q$ to denote the Hilbert space dimension of such a quantum representation of a data table - for this example $d_Q = 3$.

Proposition 1 asserts that every data table can be so constructed - that is, by pure quantum states and projective operators. That this is possible can be seen as follows. Since we are not restricted in $d_Q$, let us imagine that every preparation procedure (column of the data table) is represented by a state which is orthogonal to all the other states. That is, each state lies in its own subspace of the total Hilbert space. Clearly, if we can choose measurements so as to reproduce any desired statistics for one such state then, since the states are all orthogonal, we can piece together measurement operators for the different states in a direct sum to produce suitable measurement operators for the whole table. Focussing on one state then, imagine the measurement under consideration has outcomes occurring with probabilities $p_i$. All we need to establish is that, for a given $|\psi\rangle$, there is a way of choosing projection operators such that $\langle \psi | \Pi_i | \psi \rangle = p_i$. One way of constructing suitable operators is to work in the basis where $|\psi\rangle = |1, 0, 0, \ldots\rangle$. Let $v$ be the row vector $[\sqrt{P_1}, \sqrt{P_2}, \ldots]$, and construct the unitary matrix which has $v$ as its first row and the remaining $d-1$ rows any orthogonal basis of the support of $I - v^Tv$. Then the columns of this unitary matrix form a set of orthogonal states, and projectors onto these states satisfy $\langle \psi | \Pi_i | \psi \rangle = p_i$.

This procedure is extremely wasteful in terms of $d_Q$, the Hilbert space dimension used to represent generic data. This raises the following:

**Open Problem 1** Is there an efficient procedure for finding the smallest Hilbert space dimension required to represent an arbitrary data table in terms of pure states and projective measurements?

Although we do not have an answer to this problem, we note that being able to solve it would allow one to (approximately) solve a quantum one way communication complexity problem. Thus Open Problem 1 may benefit from studies in this field. To see the relation, note that by sending $K$ copies of systems prepared according to a procedure $P(t)$, a party Alice can have another party Bob estimate the probability of the $k$th outcome of some measurement $M(t)$ occurring. The fixed accuracy of Bob’s estimation is determined by the size of $K$. Thus, if the systems realizing the preparations and measurements consist of $n$ qubits then Alice needs to send Bob $nK$ qubits for him to obtain his estimation of the desired probability. But suppose that we consider $P(t)$ and $M(t)$ to be specified by binary strings $x_i$ and $y_j$ and denote the probability that Bob is attempting to estimate by $f(x_i, y_j)$. Then requiring Bob to perform the estimation of $f(x_i, y_j)$ with Alice sending as few qubits as possible is a quantum one way communication complexity problem. Thus the efficient procedure required by Open Problem 1 would allow us to minimize $n$ and thus (given that $K$ is a constant overhead determined only by the accuracy of Bob’s estimation) allow us to solve the associated quantum one way communication complexity problem.

The lesson of Proposition 1 is that, at its most basic level, the probabilistic structure of quantum mechanics is without physical content. To obtain such content extra assumptions or restrictions must be imposed. For example, assuming that measurements on distinct systems are described by separable (tensor products of) projection operators, the Hilbert space structure we build to yield $D$ cannot be guaranteed to reproduce all possible correlated probability distributions between multiple systems [27].

These precautions are well known but bear repeating, because in this paper we will be looking at representing a data table via a different probabilistic formalism, a formalism essentially that of classical probability theory. It is well understood that the ontological model formalism allows for an arbitrary data table to be represented - therefore our goal is to investigate more than simply whether such models can reproduce empirical observations. In fact we are primarily interested in using these models to obtain a deeper understanding of the restrictions which occur on any proposed realistic explanation for quantum mechanics. As such we will be looking at the structure of such models when they are used to model data tables corresponding to hypothetical experiments which in quantum mechanics would be described by pure state preparations and rank one projective measurements on a system of a known Hilbert space dimension. Therefore we will generally have the case that $d_Q = d$, and Open Problem 1 will not be of concern to us.
III. ONTOLOGICAL FACTORIZATION OF A DATA TABLE

A. Defining Ontological Factorizations

Our primary goal is to examine factorizations of the data matrix $D^{(x)}$, $x = 1, 2, \ldots, m$ into the product of a $d \times \Omega$ measurement matrix $M^{(x)}$ and an $\Omega \times s$ preparation matrix $P$ (both positive-real valued):

\[ D^{(x)} = M^{(x)} P, \quad \forall x = 1, 2, \ldots, m. \tag{1} \]

The columns of the preparation matrix $P$ are normalized probability distributions i.e. $P$ is column-stochastic; it satisfies $0 \leq P_{jk} \leq 1$, and $\sum_k P_{jk} = 1$ for all $j$. The interpretation of $P$ is that its $k$-th column is a (classical) probability distribution, over $\Omega$ distinct ontic states, which corresponds to the preparation procedure $P^{(k)}$ of $D$. That is, we imagine that when a system is prepared according to $P^{(k)}$, it really is prepared in one of the $\Omega$ ontic states, and our ignorance of which particular ontic state the system is in is represented by the probability distribution in column $k$ of $P$.

Each row of the measurement matrix corresponds to an indicator function over the $\Omega$ ontic states. That is, $M^{(x)}_{ij}$ is the probability of obtaining measurement outcome $i$, if the actual ontic state of the system is $j$, given that measurement $x$ is being performed.

Besides (1) there is one extra constraint on $M$, due to our desire to be able to interpret an ontological factorization as a model of the probabilistic data arising from a realistic framework. Specifically, regardless of which ontic state a system is in, one of the measurement outcomes must pertain. For instance, if we consider the $x$-th measurement performed on a system actually in ontic state $j$, then one of the $d$ outcomes must occur. As such, we need,

\[ \sum_{i=1}^{d} M^{(x)}_{ij} = 1, \tag{2} \]

for each of the $j = 1, \ldots, \Omega$. Thus the $M^{(x)}$ are also necessarily column-stochastic. This is actually an important extra constraint - without it one can reproduce quantum statistics with non-contextual ontological models not having negative indicator functions - which has been shown not to be possible by Spekkens [8]. (They would have a decidedly weird ontology however, as they would require a strange non-separable conspiracy between preparation and measurement devices.)

With the above constraints in mind, we can define an ontological factorization more formally as:

**Definition 1** A data table $D$ possesses an ontological factorization (OF) over $\Omega$ ontic states if there exists an $\Omega \times s$, column-stochastic matrix $P$, and $d$ matrices $M^{(x)}$, each $m \times \Omega$ dimensional and column-stochastic, which satisfy $D^{(x)} = M^{(x)} P$ for all $x = 1, 2, \ldots, d$.

If the entries of $M$ are all 0 or 1, then the ontological factorization is deterministic, otherwise it is indeterministic.

B. Model 1: An indeterministic ontological factorization

We now briefly present a trivial OF, which is easily performed for any data table. This will be rendered much less trivial in subsection III E. Specifically, in this OF of the data table $D$ we choose

\[ M^{(x)} = D^{(x)} \text{ and } P = 1. \]

This OF has $\Omega = s$. That is, the number of ontic states is equal to the number of preparation procedures (quantum states) used in constructing the data table. In terms of an ontological model, this OF implies that preparing a system in a quantum state $|\psi\rangle$ is equivalent to preparing the system in a single (determined) ontic state (since each column of $P$ has only one non-zero entry). In the terminology of [11] this model is $\psi$-ontic (and $\psi$-complete).

Measurements in this model are represented by indeterministic indicator functions - the model simply specifies what the probability is that a system in a given ontic state yields each outcome of any specified measurement.

This ontological model, when extrapolated to a “continuum limit” (i.e., constructed for a data table of all measurements and preparation procedures for a quantum system of some fixed Hilbert space dimension), becomes the model of Beltrammati-Bugajski [12], which was presented as example number 1 in [7]. In that model the ontological state space is simply the complex projective space, the quantum state is represented by a Dirac delta function distribution, and the indicator functions over the space are indeterministic, with probabilistic weights defined by the Born rule.

Model 1 formally encapsulates the commonly expressed viewpoint that the quantum state is the state of reality.

C. Model 2: A deterministic ontological factorization

We now turn to a deterministic OF which can be constructed for any data table. This OF has $\Omega = d^m$ ontic states. It is convenient to index the ontic states (that is, the rows of $P$ and columns of $M$) by an $m$-tuple of integers of the form $(j_1, j_2, \ldots, j_m)$ where each of the $j_x$ ranges over $1, 2, \ldots, d$. We then assign probabilities over the ontic states to create $P$ as follows:

\[ P_{(j_1, j_2, \ldots, j_m), k} = \prod_{x=1}^{m} D^{(x)}_{j_x, k}. \]

Alternatively we could specify that the $k$-th column of $P$, denoted $P_{:, k}$, is formed from the $k$-th column of $D$ as
follows:

\[ P_{i,k} = \bigotimes_{x=1}^{m} D^{(x)}_{j_x,k} . \]

Consider summing over index \( j_1 \):

\[
\sum_{j_1} P_{(j_1, j_2, \ldots, j_m),k} = \sum_{j_1} \prod_{x=1}^{m} D^{(x)}_{j_x,k} \\
= \left( \prod_{j_1=1}^{d} D^{(1)}_{j_1,k} \right) \prod_{x=2}^{m} D^{(x)}_{j_x,k} \\
= \prod_{x=2}^{m} D^{(x)}_{j_x,k}, \tag{3}
\]

since \( D^{(1)} \) is column-stochastic. We see that in general summing over an index simply removes all terms from the product which contain that index. Summing over all row indices \( j_x \) in this way we confirm that \( P \) is column-stochastic as required.

We now consider how to construct row \( i \) of \( M^{(x)} \), which corresponds to the indicator function for \( \Pi^{(x)}_i \). We assign the value 1 to every entry in this row for which the column index \((j_1, j_2, \ldots, j_m)\) has \( j_x = i \). More formally,

\[ M^{(x)}_{i,(j_1, j_2, \ldots, j_m)} = \delta_{i,j_x} . \]

To see that this works as desired, take, for example, \( i = 1 \), so we are dealing with the first row of \( M^{(x)} \). We compute the inner product of this row with the matrix \( P \):

\[
\sum_{j_1, \ldots, j_m} M^{(x)}_{i,(j_1, j_2, \ldots, j_m)} P_{(j_1, j_2, \ldots, j_m),k} \\
= \sum_{j_1, \ldots, j_m} \delta_{i,j_x} P_{(j_1, j_2, \ldots, j_m),k} \\
= \sum_{j_2, \ldots, j_m} P_{(1, j_2, \ldots, j_m),k} \\
= D^{(1)}_{1,k} \sum_{j_2, \ldots, j_m} P_{(j_2, \ldots, j_m),k} \\
= D^{(1)}_{1,k},
\]

where we have used the observation in Eq. (3) multiple times. Thus we see that we reproduce the required statistics of the data table.

An example may help illustrate the idea. Consider the following data table with \( d = 3 \) and \( m = 2 \):

\[
D = \begin{bmatrix}
0 & 2/3 \\
1/3 & 1/3 \\
2/3 & 0 \\
1/3 & 1/2 \\
1/3 & 1/2 \\
1/3 & 0
\end{bmatrix}. \tag{4}
\]

Following the construction above, the matrices \( M \) and \( P \) are given by

\[
M = \begin{pmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1
\end{pmatrix},
P = \begin{pmatrix}
0 & 1/3 \\
0 & 1/3 \\
0 & 0 \\
1/9 & 1/6 \\
1/9 & 1/6 \\
1/9 & 0
\end{pmatrix}.
\tag{5}
\]

There are two points to make about this model. Firstly, unlike Model 1, the columns of the matrix \( P \) from Model 2 are not orthogonal (disjoint). That is, the probability distributions corresponding to non-orthogonal states overlap. Such models are called \( \psi \)-epistemic in [11]. In such models, knowing the ontic state of the system does not allow one to infer with certainty what quantum state would describe the same preparation. Unfortunately, this is only true in the case of a finite data table, \( m < \infty \). In the continuum limit of this model, the probability distributions of non-orthogonal states become disjoint. To prove this rigorously requires a diversion into the infinite tensor product structures first considered by von Neumann [13], and we will not do so here. We point out, however, that even though it is \( \psi \)-ontic in the continuum limit, it is not, in the terminology of [11], \( \psi \)-complete. (A \( \psi \)-complete model would have only one ontic state consistent with any given quantum state.)

Finding models which are \( \psi \)-epistemic in the continuum limit is not easy, some attempts were given in [14], and we believe Barrett has made some recent progress [9]. Because there is a continuum of quantum states, one way to ensure an ontological model representation of all states and measurements in a Hilbert space of dimension \( d_Q \) is \( \psi \)-epistemic is simply to find a model which makes use of only a finite number of ontic states. Hardy [15] has shown that this is not possible - as the number of states and measurements increases, the number of ontic states must increase. However, Hardy’s analysis relies only on the fact that we must be able to divide the ontic state space into disjoint sets (to represent orthogonal measurements), and that as we go to the continuum limit there are an infinite number of orthogonal measurements that need to be represented in this manner [28]. Now the number of ways of dividing \( \Omega \) ontic states into disjoint sets grows exponentially. It would therefore seem that the possibility remains open that the number of ontic states required for an indeterministic model might grow only logarithmically as the size of the data table.

But in fact this is not possible. To see this, consider the simplest case of OF’s of data tables having \( d = 2 \), which we can show must satisfy the tight bound \( \Omega = \min \{ 2^m, s \} \). Clearly Models 1 and 2 set an upper bound of \( \Omega \leq \min \{ 2^m, s \} \) on the required number of on-
tic states, by providing deterministic and indeterministic factorizations having $\Omega = s$ and $\Omega = 2^m$ respectively. To give the tight bound claimed, it remains to show that for given $s$ and $m$ there always exists a data table requiring an ontological factorization having $\Omega \geq 2^m$ if $2^m \leq s$ or $\Omega \geq s$ if $s < 2^m$. We will give a general construction for a data table that lower bounds $\Omega$ and then show how it applies in the case of each of these inequalities between $s$ and $m$. First note that we can write the data tables we consider as including only the probabilities for the first outcome of each measurement (since $d = 2$ the probabilities of the second outcomes are then trivially determined). Thus we can consider a data table with some parameters $\tilde{m}$ and $\tilde{s}$ having columns made up from all $\tilde{m}$-bit binary strings. For example, if $\tilde{m} = 3$ and $\tilde{s} = 8$ then the data table thus constructed would be,

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
\end{pmatrix}
$$

But an OF of any data table of this form must employ at least $2^\tilde{m}$ ontic states. This follows since the outcomes of measurements $M_1^{(1)}, M_2^{(2)}$ and $M_3^{(3)}$ are completely determined given any of the 8 preparations shown (i.e. the relevant entries of $D$ are all $0/1$); therefore any ontic states in the supports of these preparations (i.e. assigned a non-zero value in the relevant column of an OF’s $P$ matrix) must be deterministic (take 0/1 values) with respect to these three measurements. Thus in the example given in (6), we must use at least 8 ontic states to deal with the 8 distinct possibilities for assigning outcomes to $M_1^{(1)}, M_2^{(2)}$ and $M_3^{(3)}$. Clearly, by the same reasoning, such a data table constructed with $2^\tilde{m}$ preparations will require $\Omega \geq 2^\tilde{m}$. Similarly, any data tables having general parameters $s$ and $m$ and containing sub-tables of the form (6) will require OFs with at least $2^\tilde{m}$ ontic states. Thus it only remains to determine the largest such sub-table - i.e. largest value of $\tilde{m}$ - that can fit in data tables with parameters subjected to each of the constraints $2^m \leq s$ and $2^m > s$. If we have $2^m \leq s$ then we can find a sub-table of the form (6) having $\tilde{m} = m$ and $\tilde{s} = s$, giving $\Omega \geq 2^m = \min \{2^m, s \}$. If however, $2^m > s$, then the largest sub-table of the form (6) that we can find will have $\tilde{m} = \log_2(s)$ and $\tilde{s} = s$, yielding $\Omega \geq s = \min \{2^m, s \}$. Thus in both cases the lower bound $\Omega \geq \min \{2^m, s \}$ holds. Combining this with the trivial upper bound provided by Models 1 and 2 gives the tight bound $\Omega = \min \{2^m, s \}$, showing that as the size of a data table is increased, the number of ontic states must grow faster than a logarithmic dependence on the parameters $s$ and $m$. The general question of how many ontic states are required to represent any particular given data table is taken up in Section IV.

The second point to make about Model 2 is that the number of ontic states grows exponentially with the number of measurements being performed. However, this need not always be the case, as can be seen for models in which $\Omega$ depends on $m$ by invoking Caratheodory’s theorem to yield a lower bound on $\Omega$ [29]. In the next section we explicitly demonstrate such a lower bound by introducing our final model: a deterministic ontological factorization having $\Omega = s (dm - 1)$ [30].

**D. Model 3: A deterministic ontological factorization with $\Omega = O(poly(m))$**

Our final ontological factorization is tailored to employ a number of ontic states that does not increase exponentially with the number of measurements to be described. This model is best illustrated by an example of its construction. Consider the data table from (4) (the method we outline is trivially adapted to an arbitrary data table). We deal with each column of $D$ separately. Suppose that we are attempting to reproduce the second column of $D$, corresponding to some preparation procedure $P(2)$:

$$
\begin{pmatrix}
2 \\
\frac{3}{4} \\
0 \\
\frac{1}{2} \\
0 \\
\end{pmatrix}
$$

We begin by finding the smallest entry in the chosen column, which in this case takes a value of $\frac{1}{2}$, and is associated with the second outcome of the first measurement. We then move this entry into another column vector, to be added to what remains of the original. We also remove the same value of $\frac{1}{2}$ from one of the second column entries associated with the remaining measurement - restricting our choice only to ensure that the chosen entry is greater than $\frac{1}{2}$. Referring to the second column of $D$ shown above, we see that there are two such entries to choose from, associated with the first and second outcomes of the second measurement and both taking the value $\frac{1}{2} > \frac{1}{2}$. We choose the entry associated with the first outcome, and thus obtain:

$$
\begin{pmatrix}
2 \\
\frac{1}{4} \\
0 \\
\frac{1}{4} \\
0 \\
\end{pmatrix}
+ \begin{pmatrix}
0 \\
\frac{1}{3} \\
0 \\
\frac{1}{3} \\
0 \\
\end{pmatrix}
\rightarrow \begin{pmatrix}
\frac{7}{6} \\
\frac{1}{3} \\
\frac{1}{3} \\
\frac{1}{3} \\
0 \\
\end{pmatrix}
$$

The new binary column vector we have generated provides a valid set of deterministic measurement outcomes for an ontic state (weighted by $\frac{1}{2}$). In particular, note that by subtracting the same value from a single entry associated with each measurement we have ensured that
the binary vector satisfies the stochasticity requirement of (2). We can repeatedly apply this procedure to the ‘remainder’ vector \( \left[ \frac{3}{4}, 0, \frac{1}{2}, \frac{1}{2}, 0 \right] \) on the right hand side of the above expression, until only column vectors with binary entries remain. This gives:

\[
\begin{bmatrix}
\frac{2}{3} \\
\frac{1}{3} \\
0 \\
\frac{1}{2} \\
\frac{1}{2}
\end{bmatrix} \rightarrow \frac{1}{3}
\begin{bmatrix}
0 \\
1 \\
0 \\
0 \\
0
\end{bmatrix} + \frac{1}{3}
\begin{bmatrix}
0 \\
1 \\
1 \\
0 \\
0
\end{bmatrix} + \frac{1}{2}
\begin{bmatrix}
0 \\
0 \\
1 \\
1 \\
0
\end{bmatrix}
\]

\[
= \frac{1}{3}
\begin{bmatrix}
0 \\
1 \\
0 \\
0 \\
0
\end{bmatrix} + \frac{1}{3}
\begin{bmatrix}
0 \\
1 \\
1 \\
0 \\
0
\end{bmatrix} + \frac{1}{2}
\begin{bmatrix}
0 \\
0 \\
1 \\
1 \\
0
\end{bmatrix}
\]

The three 0/1 vectors generated by this procedure can be used as valid columns of an \( M \) matrix, and we can take the associated probabilistic weightings to form a \( P \) matrix row corresponding to the preparation \( \mathcal{P}(2) \). Thus by introducing three ontic states we have formed \( P \) and \( M \) matrices that can reproduce the quantum statistics for all measurements from \( D \) performed on the single preparation \( \mathcal{P}(2) \). Repeating this process to introduce a new set of ontic states for the remaining column of \( P \) (corresponding to a preparation \( \mathcal{P}(1) \)), yields the following deterministic ontological factorization,

\[
M = \begin{bmatrix}
0 & 0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0
\end{bmatrix}, \quad P = \begin{bmatrix}
\frac{1}{4} & 0 \\
\frac{1}{4} & 0 \\
\frac{1}{4} & 0 \\
\frac{1}{4} & 0 \\
\frac{1}{4} & 0
\end{bmatrix}
\]

Note that since we introduce a whole new set of ontic states for each preparation, the entries of different columns of our \( P \) matrix are bound to be completely disjoint. Thus, following the terminology of [11], Model 3 can be classified as \( \psi \)-ontic.

The procedure outlined above will generally require introducing \( dm - 1 \) ontic states for each preparation from \( D \), which suggests \( \Omega = s(dm - 1) \). However, Model 3 often allows us to exceed this value, so long as the procedure is applied carefully, exploiting repeated entries in \( D \) to reduce the number of ontic states we need to introduce. By this token the example given above has \( \Omega = 6 \) - almost half of \( s(dm - 1) = 10 \).

E. Deterministic ontological factorizations from indeterministic ones

In this section we will examine a process for turning the indeterministic \( OF \) of Model 1 into a deterministic \( OF \). First a point of notation: from now on we will often use the two dimensional array versions of the data table and measurement matrices:

\[
D = \begin{bmatrix}
D^{(1)} \\
\vdots \\
D^{(m)}
\end{bmatrix}, \quad M = \begin{bmatrix}
M^{(1)} \\
\vdots \\
M^{(m)}
\end{bmatrix},
\]

so that the \( OF \) becomes simply \( D = MP \).

The simplest version of the procedure we outline for recovering determinism from indeterminism is most easily illustrated by an example. Consider the following data table:

\[
D = \begin{bmatrix}
1/2 & 2/3 \\
1/2 & 1/3 \\
3/4 & 1 \\
1/4 & 0
\end{bmatrix}.
\]

The \( OF \) of model 1 would have \( M = D \) and

\[
P = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}.
\]

That is, \( \Omega = 2 \). The first step is to notice that each of the probabilities in the first column of \( D \) is an integer multiple of 1/4, while each in the second column is an integer multiple of 1/3. We therefore expand the supports of the probability distributions in \( P \) from single ontic states to 4 and 3 ontic states respectively:

\[
P = \begin{bmatrix}
1/4 & 0 \\
1/4 & 0 \\
1/4 & 0 \\
0 & 1/3 \\
0 & 1/3 \\
0 & 1/3
\end{bmatrix}.
\]

Note that the probability distributions are still disjoint (in the language of [11] the model is \( \psi \)-ontic but not \( \psi \)-complete). We now want to choose a matrix \( M \) with only 0/1 entries. If we choose the first row of \( M \) (i.e. the indicator function for the first measurement outcome) to be

\[
\left( \begin{array}{ccccccc}
1 & 1 & 0 & 0 & 1 & 1 & 0
\end{array} \right),
\]
then we will certainly produce the first row of \( D \). The \( k \) is that the disjointness of the two columns of \( P \) enable us to assign 1’s and 0’s to \( M \)'s first row in an essential unrestrict fashion - the first 4 elements of this row simply need to pick up enough 1/4’s from \( P \) to give the entry 1/2 for \( \psi_1 \), and similarly the last three entries must pick up an appropriate number of the 1/3’s to give the entry 2/3 for \( \psi_2 \). Assigning the second row we need to be more careful. One assignment which naively would see to work, in as much as it would reproduce the data table entries when multiplied by \( P \), is

\[
\begin{pmatrix}
1 & 1 & 0 & 0 & 1 & 0 & 0
\end{pmatrix}.
\]

However this violates the constraint of column stochasticity on the \( M^{(x)} \)'s from Definition 1. Such \( \varepsilon \) indicator function would imply that a system in ontic state 1 gives both the first measurement outcome and the second outcome with certainty! The only choice for this row once we have chosen the first row as above is

\[
\begin{pmatrix}
0 & 0 & 1 & 1 & 0 & 0 & 1
\end{pmatrix}.
\]

Proceeding in this manner, one possibility for \( M \) is

\[
\begin{pmatrix}
1 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0
\end{pmatrix}.
\]

Imagine now that the data table only contains rational fractions as entries. This would certainly be the case if we were considering a table which was assembled from actual experimental data. Clearly, generalizing the above procedure will allow us to find \( M \) and \( P \) matrices so as to obtain a deterministic OF. This does not give us a procedure for obtaining a finite OF for any data table however, since we may wish to consider ones constructed from quantum states and projectors which have irrational valued overlaps. For the general program of research into ontological models there is no requirement of finiteness - in particular the trick of spreading the support of the probability distribution over extra ontic states can readily be performed by spreading the distribution over variables of cardinality \( 2^{8\log} \). This yields a procedure for transforming any indeterministic ontological model into a deterministic one - and is essentially what Bell did [16] (see example 4 in [7]) to provide a counterexample to ‘von-Neumann’s silly assumption’. In doing so one has increased the number of ontic states required to describe the system - the extent to which this is necessary, as opposed to merely sufficient, is an interesting question, which to some extent we take up again in Section IV.

In the last four sections we have derived a series of bounds on the number of ontic states that ontological factorizations must employ. By a simple extension of the argument given in Sec. III C we have that data tables with arbitrary parameters \( s, d, m \) require a number of ontic states that is tightly bounded by \( \Omega = \min \{ d^m, s \} \). However, the explicit construction that we gave in Sec. III D showed that by letting \( \Omega \) depend on all three parameters of a data table, the number of ontic states need not depend exponentially on \( m \). These bounds clearly have interesting repercussions for the ability to classically simulate quantum systems efficiently. For example, our lower bound \( \Omega \geq \min \{ d^m, s \} \) shows that one cannot precisely reproduce a general data tables quantum statistics by keeping track of a number of ontic states that grows only logarithmically with the number of preparations and measurements considered. Extending and refining the bounds we have presented is an interesting direction for future research, which may benefit from existing results in the literature. For example, Aaronson has shown in [17] that the probabilities for a set of \( m \) two-outcome measurements performed on an \( N \) dimensional quantum system can be approximately calculated (to some fixed accuracy) from a classical string of length \( O(\log(N) \log \log(N) \log(m)) \). This shows that a data table containing \( m \) such measurements and some set of preparations associated with an \( N \) dimensional quantum system has an approximate ontological factorization that employs \( \Omega = 2^{O(\log(N) \log \log(N) \log(m))} = m^{O(\log(N) \log \log(N))} \) ontic states (wherein each ontic state encodes a possible instance of the string one can construct to encode the required statistics). Thus, in cases where one is satisfied with approximately reproducing the entries of a data table, the results in [17] give a lower bound on \( \Omega \) which depends pseudo-polynomially on \( m \) and \( N \), but interestingly not on \( s \) (the precise number of preparations in the data table).

In Sec. IV D we will also note how existing results concerning matrix factorization problems might prove useful.
in deriving more bounds on $\Omega$.

F. Contextuality in ontological factorizations

By the famous result of Kochen and Specker [18] deterministic ontological models must be measurement-outcome contextual. We now consider how measurement outcome contextuality manifests itself in an OF of a data table. Contextuality needs to be considered when different quantum measurements share a common projector. In such a case a data table might look something like (with $d = 3$):

\[
\begin{bmatrix}
0.08 & 1 & 0.67 & 0.09 \\
0.51 & 0 & \ldots & \ldots \\
0.41 & 0 & \ldots & \ldots \\
0.08 & 1 & 0.67 & 0.09 \\
0.92 & 0 & \ldots & \ldots \\
0.00 & 0 & \ldots & \ldots 
\end{bmatrix}.
\]

(7)

Rows 1 and 4 contain the same entries, and so in quantum mechanics they could correspond to measurement outcomes represented by the same projector. Initially one might have been tempted to simply exclude the redundant rows. The essence of the Kochen-Specker theorem is that doing so would prevent us being able to explain the data table in terms of a deterministic ontological model, and so we retain them. It is at this point that we depart from the $r$-p formalism. In the $r$-p formalism there is a unique $r$-vector for each quantum projector. As mentioned above, this presumption of measurement outcome non-contextuality is the reason the $r$-vectors require negative entries (or entries greater than 1)[31].

In terms of our OF’s, the contextuality required by the Kochen-Specker theorem manifests itself as follows: If two rows of the data table are identical, then one cannot necessarily find an OF such that the two corresponding rows of $M$ are identical. Now, if the only constraint on the factorization was that $D = MP$ with $M$ a 0/1 matrix, then this would not be true, since there would be nothing stopping the replacement of one of those rows of $M$ by the other. The key issue, as mentioned above, is the extra column-stochasticity constraint on the factorization, which forces at least one measurement outcome to be obtained for any given ontic state.

Let us demonstrate all this with an example. In [19] Kernaghan provided an example of a set of measurements in a 4 dimensional Hilbert space for which a Kochen-Specker obstruction exists (see also [20]). These measurements are built from the following 20 states in a Hilbert space of dimension 4 (the normalization factors of $1/\sqrt{2}$ or $1/2$ are omitted, and $\bar{I}$ denotes $-1$):

\[
\begin{align*}
|\psi_1\rangle &= (1\ 0\ 0\ 0),
|\psi_{11}\rangle &= (1\ 1\ 1\ 1),
|\psi_2\rangle &= (0\ 1\ 0\ 0),
|\psi_{12}\rangle &= (1\ \bar{I}\ \bar{I}\ 1),
|\psi_3\rangle &= (0\ 0\ 1\ 0),
|\psi_{13}\rangle &= (1\ 1\ \bar{I}\ \bar{I}),
|\psi_4\rangle &= (0\ 0\ 0\ 1),
|\psi_{14}\rangle &= (0\ 1\ 1\ 0),
|\psi_5\rangle &= (0\ 0\ 1\ 1),
|\psi_{15}\rangle &= (0\ 1\ \bar{I}\ 0),
|\psi_6\rangle &= (0\ 0\ 1\ \bar{I}),
|\psi_{16}\rangle &= (1\ 0\ 0\ \bar{I}),
|\psi_7\rangle &= (1\ \bar{I}\ 0\ 0),
|\psi_{17}\rangle &= (\bar{I}\ 1\ 1\ 1),
|\psi_8\rangle &= (0\ 1\ 0\ 1),
|\psi_{18}\rangle &= (1\ \bar{I}\ 1\ 1),
|\psi_9\rangle &= (1\ 0\ 1\ 0),
|\psi_{19}\rangle &= (1\ 1\ \bar{I}\ 1),
|\psi_{10}\rangle &= (0\ 1\ 0\ \bar{I}),
|\psi_{20}\rangle &= (1\ 1\ \bar{I}\ 1).
\end{align*}
\]

The 11 sets of 4-outcome measurements which lead to a Kochen-Specker obstruction can be tabulated as follows:

\[
\begin{bmatrix}
1 & 1 & 1 & 1 & 17 & 17 & 18 & 19 & 15 & 6 & 9 \\
2 & 2 & 3 & 4 & 18 & 19 & 20 & 16 & 7 & 8 \\
3 & 5 & 8 & 14 & 19 & 9 & 14 & 5 & 11 & 11 & 13 \\
4 & 6 & 10 & 15 & 20 & 10 & 16 & 7 & 12 & 13 & 12
\end{bmatrix}.
\]

(8)

So, for example, the third measurement $\Pi^{(3)}$ consists of the projectors $\{|\psi_1\rangle\langle\psi_1|, |\psi_2\rangle\langle\psi_2|, |\psi_3\rangle\langle\psi_3|, |\psi_4\rangle\langle\psi_4|\}$. The proof that these projectors cannot be assigned a unique truth value (i.e. independent of the other projectors in the measurement) is trivial. In each of the odd number (i.e. 11) of measurements, only one projector can (and must) be assigned the truth value 1. This is in direct conflict with the fact that each of the $|\psi_i\rangle$’s appears an even number of times in (8).

The data table for these 11 measurements and the 20 states is depicted in a color coded fashion in Figure 1. Applying the procedure of section III E allows us to generate matrices $M$ and $P$ for a deterministic OF over $20 \times 4 = 80$ ontic states. The matrices for this OF are depicted in Figure 2.

An example of the contextuality of this OF can be seen by considering rows 3 and 10, which correspond to the same measurement projector $|\psi_3\rangle\langle\psi_3|$ (these rows are marked on $M$ in Figure 2 by red arrows). Clearly each of these indicator functions must have a 1 at all of the set of ontic states which $|\psi_3\rangle$ has support over (c.f. the third column in $P$ - that is, ontic states 10 through 13). We see, however, that there are some ontic states (71, 75 and 79 for example) that do not lie in the support of $|\psi_3\rangle$, and to which one of rows 3 or 10 assigns a 1 while the other assigns a 0. Ontic states such as 71, 75 and 79 also show that there are some ontic states which are assigned a value 1 by the row in $M$ corresponding to $|\psi_3\rangle\langle\psi_3|$ but not by the column in $P$ corresponding to $|\psi_3\rangle$. As discussed in [7] this is a general (necessary) feature of all ontological models: there are necessarily some ontic states which pass a test $|\psi\rangle\langle\psi|$ for a system “being in” a state $|\psi\rangle$, which can never be prepared when the preparation procedure specifies the quantum state to be
FIG. 2: (Color online) P and M matrix for a deterministic OF of the Kernaghan set of preparations and measurements. The black squares denote a value of 1, the red of 1/4 whilst the white squares represent 0.

$|\psi\rangle$. This asymmetry of deterministic ontological models between preparations and measurements, which is not present in quantum mechanics, was termed deficiency in [7]. The terminology comes from the fact that the support of the probability distribution corresponding to the quantum state is strictly less than the support of the indicator function corresponding to a projection onto that state, as we have seen. We term unfaithful those ontic states which do not lie in the support of the probability distribution, but which do pass the test (since for some measurements they will “choose” to give a different outcome). Note that if an ontological model is therefore to be able to describe preparing the state $|\psi\rangle$ by performing a measurement of $|\psi\rangle\langle\psi|$, it is going to be the case that a system in an unfaithful ontic state must be disturbed by the measurement in order to end up in one of the faithful states.

IV. ONTOLOGICAL COMPRESSION

So far we have investigated OF’s without particular regard to how large the number of ontic states $\Omega$ is required to be. In this section we consider the problem of trying to either find OF’s with $\Omega$ as small as possible, or to reduce the value of $\Omega$ for a given OF - a process we call “ontological compression”. Such a reduction in ontic states clearly has repercussions for the ability to efficiently simulate quantum systems classically - a point we elaborate on in Sec. IV C. But, as we shall see, our ontological compression schemes also provide routes towards constructing $\psi$-epistemic models in which we can truly view the quantum description of a system as a state of knowledge.

Models 1 and 2 gave OF’s which require $\Omega = s$ and $\Omega = dm$ respectively - these values set upper bounds on $\Omega$ for indeterministic and deterministic OF’s respectively. But since deterministic ontological factorizations can be seen as a special case of indeterministic ones then Model 2 also provides an upper bound of $\Omega = dm$ for indeterministic factorizations. There are therefore upper bounds on $\Omega$ for both deterministic and indeterministic models which depend only on data tables measurements, and upper bounds for indeterministic models which depend on only $s$. One may therefore wonder whether an upper bound can be found for deterministic models which depends only on $s$. But this is not possible; a deterministic ontological factorization always requires at least $dm + 1$ ontic states.

To see why, note that each ontic state, $\lambda_i$, from a deterministic model is associated with a length $dm$ binary string, given by the $i^{th}$ column of the models $M$ matrix. Thus the ontic states of any deterministic ontological factorization can be thought of as column vectors, $\vec{\lambda}_i$, ...
defining vertices on a unit hypercube of dimension \( dm \); \( \mathcal{C}^{dm} \subset [0,1]^{dm} \). Now consider how such a model reproduces the \( k \)th column of the data table \( D \) (corresponding to the measurement statistics for some preparation \( \mathcal{P}^{(k)} \)) in terms of these \( \mathcal{X}_i \) column vectors. Writing the relevant column of \( D \) as a vector \( \vec{p}^{(k)} \in [0,1]^{dm} \) containing the outcome probabilities for each measurement, its entries are reproduced by a convex combination of the \( \vec{\lambda}_i \),

\[
\sum_{i=1}^{\Omega} q_i^{(k)} \vec{\lambda}_i = \vec{p}^{(k)}.
\] (9)

Where we use \( q_i^{(k)} \) to denote the \( i \)th element of the \( k \)th column of the OFs \( P \) matrix. Thus deterministic models can be thought of as reproducing \( D \) by convexly summing over a set of \( \Omega \) points in a \( dm \) dimensional space. But at least \( dm + 1 \) such points must be convexly summed for us to be able to represent an arbitrary point from \([0,1]^{dm}\). Thus we require at least \( dm + 1 \) columns of \( M \), i.e. at least \( dm + 1 \) ontic states.

We can also set a trivial lower bound on \( \Omega \):

**Proposition 2** Any ontological factorization must be such that \( \Omega \geq \text{rank}(D) \).

This follows immediately from the fact that \( D = MP \), the ranks of \( M,P \) cannot exceed \( \Omega \), and for general matrices \( \text{rank}(AB) \leq \min(\text{rank}(A),\text{rank}(B)) \).

As an example of where this bound can be attained in a deterministic OF, consider the data table:

\[
D = \begin{bmatrix}
1 & 0 & 1/2 & 1/2 & 1/2 & 1/2 \\
0 & 1 & 1/2 & 1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & 1 & 0 & 1/2 & 1/2 \\
1/2 & 1/2 & 0 & 1 & 1/2 & 1/2 \\
1/2 & 1/2 & 1 & 1/2 & 1/2 & 1 \\
1/2 & 1/2 & 1/2 & 1/2 & 0 & 1
\end{bmatrix}
\] (10)

This is the data table for a qubit, where the measurements are the projectors onto the eigenbases of the Pauli \( X,Y,Z \) matrices, and the states are simply the eigenstates of these three operators. This data table has the following OF:

\[
M = \begin{pmatrix}
1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 \\
0 & 1 & 1 & 0
\end{pmatrix}, \quad P = \frac{1}{2} \begin{pmatrix}
1 & 0 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & 1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 1 & 0
\end{pmatrix}
\] (11)

This OF has \( \Omega = 4 \), which is less than both \( s = 6 \) or \( d^m = 8 \), and which happens to be the rank of \( D \). (Note that this OF is equivalent to a single toy-bit of Spekkens [1].)

### A. Ontological compression: Method 1

The first technique for ontological compression we consider can be applied to any OF, but finds particular utility in compressing the deterministic OF’s generated from Model 1 (discussed in Section III E). The key is to consider the possibility that two columns \( j \) and \( j' \) of \( M \), corresponding to ontic states associated with distinct and non-orthogonal quantum states, are identical. If this is the case, then one of the ontic states is redundant, since any row of \( P \) (i.e. any quantum state) which has support at \( j' \), could just as well reproduce the relevant statistics in \( D \) by instead having support at \( j \).

For example, consider the data table given in (10) and suppose that we started with a deterministic un-compressed OF of the kind discussed in section III E so that,

\[
M = \begin{pmatrix}
1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\
0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0
\end{pmatrix}, \quad (12)
\]

\[
P = \frac{1}{2} \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\] (13)

We can immediately see that several of the columns of (12) are already equal (specifically, columns 1 and 5, 2 and 7, 3 and 12 and 4 and 10). We can therefore compress the pairs of associated ontic states together. In general however we may not be so fortunate, and we will need to manipulate the columns of \( M \) to try and make as many identical as possible. So long as we respect the constraints imposed by stochasticity and the requirement \( MP = D \) we are free to alter the entries of \( M \) as is convenient. In particular, we can change which ontic states a given indicator function (i.e. row of \( M \)) uses to reproduce any quantum states statistics within \( D \) so long as we respect the requirement that one and only one outcome of each PVM should ever occur. Consider the
$2 \times 2$ boxes we have drawn on $M$ in (12). These partition rows corresponding to distinct PVM measurements and sets of ontic states (columns) associated with different preparations [32]. In terms of these boxes, the allowed manipulations of $M$ correspond to flipping the columns of a box,

$$
\begin{bmatrix}
  a & b \\
  c & d \\
\end{bmatrix} \rightarrow \begin{bmatrix}
  b & a \\
  d & c \\
\end{bmatrix}.
$$

As an example of how one can use this freedom to compress two ontic states, columns 3 and 6 of (12) can be made equal by simply applying this permutation to the bottom box containing columns 5 and 6 (shown in red). There is however, a subtlety in forcing columns of $M$ to be equal in this way. The permutation we apply to make columns 3 and 6 equal will of course also alter column 5. But initially this column was already equal to column 1. To retain this initial equality we must apply the same permutation to the bottom box containing columns 1 and 2 (shown in blue). However, this in turn will alter column 2, which was initially identical to column 7 and so to retain this equality we must then permute the bottom box containing columns 7 and 8 (shown in green). Performing these three permutations we obtain the following new expression for $M$,

$$
M = \begin{pmatrix}
  1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
  0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\
  1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\
  0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
  1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
  0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\
\end{pmatrix}.
$$

Combined with (13) this reproduces the statistics from $D$. Counting identical columns we find that in fact there are now 8 redundant columns in $M$, three more having appeared due to the extra reshuffling we needed to perform in order to share columns 3 and 6. These redundant columns can be removed, which results in us compressing the four triples $(1, 5, 9)$, $(2, 7, 11)$, $(3, 6, 12)$, $(4, 8, 10)$ into four ontic states. We can then finally update $P$ to represent this compression by combining its rows corresponding to each of the four triples of ontic states. The resultant compressed OF is in fact precisely the optimally compressed model given in (11).

In cases with larger data tables, the compression is not quite so trivial. The Kernaghan OF for example, requires one to keep track of eighty ontic states. By applying an algorithm for randomly combining ontic states according to a natural generalization of the example given above, we are able to compress the Kernaghan OF to use only 42 ontic states. This is much lower than the $d^m$ ontic states needed by Model 2 and almost half the number required by our deterministic rendering of Model 1. The resulting $M$ and $P$ matrices are shown in Figure 3. Clearly the columns of the matrix $P$ associated with this compressed OF are not disjoint, and consequently the OF is $\psi$-epistemic. In fact, the approach to compression outlined above will always result in a $\psi$-epistemic model. It should be noted however, that the compression illustrated in Figure 3 is not guaranteed to be optimal, since it does not saturate the bound given in Proposition 2. In general, one would expect the amount by which one can compress an OF using this approach to depend on the initially chosen $M$ (picked at random for the above examples) and the order in which one chooses to compress the various ontic states of the model. Optimizing these choices is highly non-trivial.

### B. Ontological compression: Method 2

The second method for ontological compression we consider is designed to effect a compression for OF’s based on Model 2. It is also most easily illustrated by an example. Let us return to the example of Eqs. (4) and (5), reproduced here:

$$
\begin{pmatrix}
  0 & 2/3 \\
  1/3 & 1/3 \\
  2/3 & 0 \\
  1/3 & 1/2 \\
  1/3 & 1/2 \\
  1/3 & 0 \\
\end{pmatrix} = \begin{pmatrix}
  1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
  0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
  0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \\
  0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
  0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\
\end{pmatrix}.
$$

It is convenient to view the 9 entries corresponding to each of the two columns of $P$ as probability distributions over 9 “ontic state boxes” as follows:

$$
\mathbf{p}^{(1)} = \begin{pmatrix}
  0 & 1/9 & 2/9 \\
  0 & 1/9 & 2/9 \\
\end{pmatrix}, \quad \mathbf{p}^{(2)} = \begin{pmatrix}
  1/3 & 1/6 & 0 \\
  1/3 & 1/6 & 0 \\
  0 & 0 & 0 \\
\end{pmatrix}.
$$

The indicator functions are all of the form

$$
\begin{pmatrix}
  1 & 0 & 0 \\
  1 & 0 & 0 \\
  1 & 0 & 0 \\
\end{pmatrix}, \quad \begin{pmatrix}
  1 & 1 & 1 \\
  0 & 0 & 0 \\
  0 & 0 & 0 \\
\end{pmatrix}, \quad \text{etc.}
$$

That is, the construction of Model 2 is such that summing $\mathbf{p}^{(k)}$ along a column of the boxes yields the probability for the corresponding outcome of the first measurement, summing along a row yields the same for the second measurement. Thus it is clear that if we leave the row and column box-sums invariant we can “shift around” the probability weightings that the distributions $\mathbf{p}^{(1)}, \mathbf{p}^{(2)}$ assign to the ontic states. If we then find that both distributions assign a weighting 0 to an ontic state, it can be removed completely and some ontological compression has been
achieved. In fact, we already see that $P^{(1)}_{3,1} = P^{(2)}_{3,1} = 0$, and so this ontic state could be removed.

In order to shift around the probability, one simple operation involving 4 ontic states is to map them as follows:

$$
P_{i,j} \rightarrow 0, \quad P_{i,j'} \rightarrow P_{i,j'} + P_{i,j}, \quad P'_{i,j} \rightarrow P'_{i,j} + P_{i,j}, \quad P'_{i,j'} \rightarrow P'_{i,j'} - P_{i,j}.
$$

Since the final state must be a suitable probability distribution, we require $P'_{i,j'} > P_{i,j}$. In our example we can use this to implement:

$$
P^{(1)}_{2,2} \rightarrow 0, \quad P^{(2)}_{2,2} \rightarrow 0, \quad P^{(1)}_{3,3} \rightarrow 3/9, \quad P^{(2)}_{3,3} \rightarrow 1/2, \quad P^{(1)}_{3,2} \rightarrow 3/9, \quad P^{(2)}_{3,2} \rightarrow 1/3, \quad P^{(1)}_{3,3} \rightarrow 1/9, \quad P^{(2)}_{3,3} \rightarrow 1/6.
$$

In this manner we nullify weighting of both distributions on the middle ontic state (i.e. $P^{(k)}_{2,2} = 0$), and it too could be removed:

$$
P^{(1)} = \begin{bmatrix}
0 & 1/9 & 2/9 \\
0 & \mathbf{3/9} & \mathbf{3/9} \\
\mathbf{3/9} & 1/9 & 0
\end{bmatrix}, \quad P^{(2)} = \begin{bmatrix}
1/6 & 1/3 & 0 \\
1/2 & \mathbf{0} & \mathbf{0} \\
\mathbf{0} & \mathbf{0} & \mathbf{0}
\end{bmatrix}.
$$

(Where $\mathbf{0}$ denotes entries to be deleted.)

C. Classical simulation and ontological compression

We have seen that some sort of ontological compression may be possible, depending on specifics of the data tables involved. Why might one be interested in ontological compression? Consider a “family” of data tables - that is a set of data tables constructed from an increasing number of states and measurements. An example might be data tables constructed from the family of all stabilizer states on $n$-qubits, for increasing values of $n$. If it were the case that this data table can be ontologically compressed such that $\Omega$ only grows polynomially with $n$, then an efficient classical simulation of that family of states and measurements is clearly possible. If we denote by $D_n$ the data table for all $n$-qubit stabilizer states/measurements so that $D_n$ has $O(4^n)$ rows/columns (and $D_1$ would then be the data table of (10)), then we are asking whether there exists an ontological factorization of $D_n$ which has $\Omega = O(\text{poly}(n))$. But we can immediately see that this cannot be achieved, because any table containing all stabilizer states and measurements will contain a sub-table in which (for $d = 2$) $2^n$ preparations are associated with all $n$ bit strings over $n$ measurements - i.e. a sub-table of the form shown in (6). Since we have already seen that such a table will require $\Omega \geq 2^n$, then its existence clearly prohibits us from finding ontological factorization of the stabilizer data table having $\Omega = O(\text{poly}(n))$.

Actually, a polynomial sized number of ontic states is too strong a requirement for efficiency: Classical Monte-Carlo simulations, for example, can be provably efficient for certain problems even when the number of ontic states grows exponentially. Since our ontological models are also essentially classical probability representations, we similarly expect a polynomial requirement to be too strong for them.
D. Connections to other matrix factorization problems

We conclude this section with a brief discussion of how finding OF’s is related to other matrix factorization problems. Our data tables are generally not square. However, in instances where (such as in the example of Eqs. (10) and (11)) we use the same quantum states to specify both the preparation procedures and the measurements, then $D$ is symmetric, with non-negative entries, and positive semi-definite (ie doubly non-negative). These conditions are necessary (though not sufficient) for the matrix $D$ to be completely positive - that is, factorizable into a product of the form $A = B^\dagger B$, where the elements of $B$ are non-negative. Completely positive matrices have been much studied (see e.g. [22]), in particular with regards to finding (bounds on) the smallest row-dimension of $B$ for which this factorization is possible (called the “cp-rank” of $B$, or sometimes the “factorization index”).

A completely positive matrix factorization (i.e. one of the form $D = B^\dagger B$) is not generally equivalent to our OF’s. However, we have already seen an example of such a factorization appearing as an OF - the matrices $M, P$ of the example in Eqs. (10) and (11) differ only by an overall multiplicative factor of $1/2$, and so we can see this example as providing a completely-positive matrix factorization of this particular $D$. Now it is interesting to note that there is an upper bound [33] on the cp-rank [23] which is polynomial in $\text{rank}(D)$, which, in turn, is polynomial in $d_Q$. The cp-rank is, in the OF picture, the number of ontic states $\Omega$. Thus it seems plausible there exist some interesting data table families which have polynomial (in $d_Q$) sized OFs.

There is a second type of matrix factorization which has some connection to the OFs we have been considering: the so-called “non-negative matrix factorization” (NMF). In this factorization a matrix of (non-negative-valued) image data $V$ is factorized into the product of two matrices $W, H$ with non-negative elements:

$$V = WH.$$ 

NMF is often considered from the viewpoint of image compression, where the goal is to obtain an approximate factorization where $W$ ($H$) have as small a number of rows(columns) as possible. Some particularly simple procedures for performing this approximate factorization, guaranteed to converge to a local optima (with respect to various matrix distances between the ideal $V$ and the approximate one), were given in [24]. It was shown recently in [25] that if one considers optimizing with respect to the Kullback-Leibler distance, then the local optima preserve the row and column sums of the original matrix. In particular, if we consider the separate NMF factorizations

$$D^{(x)} = M^{(x)} P,$$

so $D^{(x)}$ is column-stochastic, then the results of Corollary 2 in [25] imply that the NMF found will be such that $M^{(x)}, P$ are column stochastic as we require. Of course our problem requires finding many such factorizations with the same $P$ for the $m$ different $D^{(x)}$’s. Interestingly, one reason that NMF is useful in image analysis is that it breaks the image up into “hidden variables” (Lee and Seung’s terminology, not ours!) such that an image is comprised of pieces which humans recognise as familiar fundamental components (the ears, nose and mouth of a facial image for example). This is unlike the more standard principal component analysis route to “eigenimage” compression. In these terms the OF we are considering is asking an interesting question regarding factorizing many different images (the $D^{(x)}$’s) using the same set of fundamental component images (the $P$).

V. CONCLUSIONS

By using an ontological formalism to describe finite sets of preparations and measurements performed on a quantum system we have illustrated how many features of ontological models are manifested in such discretized scenarios. We have shown how contextuality and deficiency appear in this formalism and have also been able to use the formalism to build a $\psi$-epistemic model of a discrete set of quantum statistics. We have also seen how any indeterministic description of a finite data table can be developed into an equally valid deterministic one and noted that the same technique (first employed by Bell) can be applied in the continuum limit. We have also discussed how OFs can be used to compress the number of ontic states needed to describe such discretized quantum scenarios and speculated on repercussions which this might have for classical simulations of quantum systems.

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[26] For the majority of this paper we will ignore ‘transformation procedures’ (intermediate evolutions) which are also commonly considered.
[27] Of course much deeper physical content of quantum mechanics derives from the symmetries and the Hamiltonians by which it correctly encapsulates the dynamics of the world around us.
[28] Hardy’s analysis does not actually include contextual measurements, nor does it distinguish between sets of ontic states corresponding to \( |\psi\rangle \) or those yielding outcome \( |\psi\rangle\langle\psi| \) (i.e. deficiency). However these are easily incorporated and the conclusions remain unchanged.
[29] To apply Caratheodory’s theorem in lower bounding a deterministic ontological factorization’s number of ontic states one must note that each ontic state in such a factorization is specified by a binary vector (the associated row of \( M \)), and that the entries of \( D \) are generated by convex combinations of these strings (with coefficients given by the columns of \( P \)).
[30] It may seem that the number of ontic states used by Model 3 contradicts our previous lower bound of \( \Omega \geq \{2^n, s\} \) when \( 2^n \leq s \). But note that in this case we have \( \Omega \approx s \geq 2^n \).
[31] In fact they generically have negative entries even when the data table being reproduced does not require a non-contextual representation.
[32] These sets of ontic states are guaranteed to be disjoint since Model 1 is \( \psi \)-ontic.
[33] Note that if we are interested in data tables constructed from quantum states \( |\psi\rangle \) and rank 1 operators \( |\phi\rangle\langle\phi| \) in a fixed Hilbert space dimension \( d_Q \), then finding such non-trivial upper bounds on \( \Omega \) cannot be achieved by simply finding a family of data tables of continually increasing rank and using Proposition 2. This is because \( \text{rank}(D) \leq d_Q^2 \). (To see this, note that \( D = C \circ C^* \) where \( C_{ij} = \langle \phi_i | \psi_j \rangle \)) and \( \circ \) denotes the Hadamard (elementwise) product - the result follows from standard results regarding this product \([21]\) and from the fact that \( \text{rank}(C) \leq d_Q \).)