Efficient Hidden-Variable Simulation of Measurements in Quantum Experiments

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We prove that the results of a finite set of general quantum measurements on an arbitrary dimensional quantum system can be simulated using a polynomial (in measurements) number of hidden-variable states. In the limit of infinitely many measurements, our method gives models with the minimal number of hidden-variable states, which scales linearly with the number of measurements. These results can find applications in foundations of quantum theory, complexity studies and classical simulations of quantum systems.

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In classical physics, the position and momentum of a particle determine the outcomes of all possible measurements that can be performed upon it. They define a deterministic classical state. If the state is not fully accessible, a general probabilistic classical state is a mixture of the deterministic states, arising from the inaccessibility. Since quantum mechanics gives only probabilistic predictions, it was puzzling already to the fathers of the theory whether it can be completed with an underlying classical-like model [2]. The quantum probabilities would then arise from an inaccessibility of some hidden variables (HV) describing analogs of deterministic classical states, the hidden-variable states, which determine the results of all quantum measurements.

Since the seminal work of Kochen and Specker (KS), it has been known that HV models must be contextual [2]. On the operational level, the contextual HV models cannot be distinguished from quantum mechanics. However, one may ask how plausible these models are in terms of resources, e.g., how many HV states (also called the “ontic states” [3, 4, 5]) they require. In addition to the fundamental question of the minimal HV model for a quantum system, this research is motivated by problems in quantum information theory. In particular, HV models allow a fair comparison between complexities of quantum and classical algorithms [6, 7], as a quantum algorithm can now be represented by a classical circuit.

For an infinite number of measurement settings, already a single qubit requires infinitely many HV states, the result proved by Hardy [8] and, in a different context, by Montina [9, 10]. However, these authors did not consider the scaling of the number of HV states with the number of measurements. Harrigan and Rudolph found a deterministic HV model that requires exponentially many HV states to simulate results of the finite set of measurements on all quantum states [11]. Our construction also provides such models and consumes at most a polynomial number of HV states, bringing exponential improvement. In the limit of infinitely many measurements, the number of HV states for an indeterministic model scales linearly with the number of measurements. Moreover, the number of real parameters that specify these HV states saturates the lower bound derived by Montina [10] and, consequently, is the minimal number possible. Our method also allows a universal generalization of the Spekkens model [5].

Consider a finite number, \( N \), of projective measurements on a \( d \)-level quantum system in a state \( \rho \). The probability to observe the \( r \)th result in the \( n \)th measurement is \( p^{(n)}_r(\rho) = \text{Tr}[\rho \Pi^{(n)}_r] \), where \( \Pi^{(n)}_r \) is a projector on the \( r \)th orthogonal state of the \( n \)th measurement, i.e., \( r = 1, \ldots, d \) and \( n = 1, \ldots, N \). We form a \( d \)-dimensional vector, \( \mathbf{p}^{(n)} = (p^{(n)}_1, \ldots, p^{(n)}_d)^T \), composed of the probabilities for distinct outcomes in the \( n \)th measurement. For the set of measurements, we build a \( dN \)-dimensional preparation vector, \( \mathbf{p} = (\mathbf{p}^{(1)}, \ldots, \mathbf{p}^{(N)})^T \) [12]. The deterministic HV states predetermine the results of all measurements and can be represented as a \( dN \)-dimensional vector

\[
\mathbf{O}_{r_1 \ldots r_N} = (0, \ldots, 1, \ldots, 0) \ldots (0, \ldots, 1, \ldots, 0)^T, \quad (1)
\]

where \( r_n \) is the position of 1 in the \( n \)th sequence (\( r_n = 0, \ldots, d - 1 \) indicates that outcome \( r_n \) occurs in the \( n \)th measurement). The space of all HV states, \( \Lambda \), is formed by classical mixtures of \( d^N \) deterministic states \( \mathbf{O}_{r_1 \ldots r_N} \).

A set of \( \kappa \) quantum states \( \rho_1, \ldots, \rho_\kappa \) has a HV model for \( N \) measurements, if one can find \( L \) vectors \( \mathbf{O}_1, \ldots, \mathbf{O}_L \in \Lambda \) such that

\[
\mathbf{p}(\rho_k) = \sum_{l=1}^L \alpha_l(k) \mathbf{O}_l, \quad \text{for all } k = 1, \ldots, \kappa \quad (2)
\]

where \( \alpha_l(k) \geq 0 \) and \( \sum_{l=1}^\kappa \alpha_l(k) = 1 \). The model is called deterministic if all \( \mathbf{O}_l \) are deterministic HV states; otherwise, it is called indeterministic. The model is preparation-universal, if the HV states simulate any physical state \( \rho \), and it is measurement-universal if they simulate any measurement.
Bloch sphere. The preparation vector for these directions is described by a 2-ball \(|p|\) of states. The expansion coefficients are where the columns of the displayed matrix are the \(HV\) vectors for the measurement \(x\) for the + direction. For a given preparation vector \(x\), for the \(+\) \(m\) direction, one can reduce ("compress") the preparation vector to \(p(x) = (\frac{1+mx}{2}, \frac{1-mx}{2})\). Similarly, the deterministic \(HV\) states are reduced to \(N\)-dimensional vectors \(O_{1\ldots N} = (r_1, \ldots, r_N)^T\), where \(r_n = 0, 1\). The (reduced) space \(\Lambda\) is a hypercube in \(N\) dimensions, with \(2^N\) vertices defined by these states. By Carathéodory’s theorem [15] for each vector \(p(x) = (p_1, \ldots, p_N)^T\), one can identify \(N + 1\) \(HV\) states the convex hull of which contains \(p(x)\). For a given \(x\), the vector \(p(x)\) can be written as a permutation of a reordered preparation vector \(p^\dagger(x)\) wherein the probabilities appear in increasing order, \(p_1^\dagger \leq p_2^\dagger \leq \cdots \leq p_N^\dagger\), and the latter can be expressed in terms of \(N + 1\) \(HV\) states as

\[
p^\dagger(x) = \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 \\
0 & 1 & 1 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 1 & 1 & 1 & \cdots & 1
\end{pmatrix}
\begin{pmatrix}
\alpha_0 \\
\alpha_1 \\
\alpha_2 \\
\vdots \\
\alpha_{N-1} \\
\alpha_N
\end{pmatrix},
\]

(3)

where the columns of the displayed matrix are the \(HV\) states. The expansion coefficients are

\[
\alpha_0 = 1 - p_N^\dagger, \quad \alpha_1 = p_1^\dagger,
\]

\[
\alpha_n = p_n^\dagger - p_{n-1}^\dagger \quad \text{for} \quad n = 2, \ldots, N.
\]

(4)

and, due to the ordering of probabilities, the coefficients are all positive and sum up to 1. One can suitably permute the rows in matrix given by (3) to bring the probabilities in order given by \(p(x)\). Thus, \(p(x)\) can be written as a convex combination of \(N + 1\) columns (\(HV\) states) of a reordered matrix. The number of \(N + 1\) states can be further reduced. E.g., for two equal probabilities, \(p_1 = p_2\), the number of \(HV\) states is decreased because \(\alpha_2 = 0\). If, say, \(p_2 = 1 - p_1\), one can exchange \(m_1 \rightarrow -m_1\), such that the probabilities become equal, leading to another reduction. Importantly, different quantum states are generally modeled by different sets of \(N + 1\) \(HV\) states.

As an illustrative example, consider a model for three complementary measurements along \(m_x, m_y, m_z\). We show a nonuniversal model, only for the eigenstates of these measurements: \(\pm m_x, \pm m_y, \pm m_z\). The corresponding preparation vectors are: \(p_x^+ = (1, 1, 1)\), \(p_x^- = (0, 0, 1)\), \(p_y^+ = (1, 1, 1)\), \(p_y^- = (0, 0, 1)\), and \(p_z^+ = (1, 1, 1)\), \(p_z^- = (0, 0, 1)\). Applying the method of [9] to each of these preparation vectors, one finds that \(L = 4\) \(HV\) states are sufficient for the simulation: \(O_0 = (1, 1, 1)^T\), \(O_1 = (1, 0, 0)^T\), \(O_2 = (0, 0, 1)^T\), and \(O_3 = (0, 1, 1)^T\). These four states, together with their decomposition of the preparation vectors,

\[
p_x^+ = \frac{1}{2} O_0 + \frac{1}{2} O_1, \quad p_x^- = \frac{1}{2} O_2 + \frac{1}{2} O_3,
\]

\[
p_y^+ = \frac{1}{2} O_0 + \frac{1}{2} O_2, \quad p_y^- = \frac{1}{2} O_1 + \frac{1}{2} O_3,
\]

\[
p_z^+ = \frac{1}{2} O_0 + \frac{1}{2} O_3, \quad p_z^- = \frac{1}{2} O_1 + \frac{1}{2} O_2.
\]

(5)

are equivalent to the toy model of Spekkens [5].

We give a constructive proof that a preparation-universal simulation of \(N\) quantum measurements on a qubit can be achieved with the number of \(HV\) states that is polynomial in \(N\). Let \(M\) denote a polytope formed as a convex hull of the measurement settings, \(M = \text{conv}\{\pm m_1, \ldots, \pm m_N\}\). Its dual polytope is a set

\[
D_M = \{y \in \mathbb{R}^3 | -1 \leq m_n y \leq 1, n = 1 \ldots N\}.
\]

(6)

The polytope \(M\) lies inside the Bloch sphere and its dual contains the sphere. Therefore, every Bloch vector can be written as a convex combination of the vertices, \(y_i\), of the dual polytope, \(x = \sum_i \alpha_i(x) y_i\). The components of the measurement vector can now be decomposed as \(p_n(x) = \sum_i \alpha_i(x) \frac{1}{2} (1 + m_n y_i)\). According to the definition of the dual polytope, the quantity \(\frac{1}{2} (1 + m_n y_i) \in [0, 1]\) and can be interpreted as the \(n\)th component (probability) of the \(i\)th \(HV\) state. Since the Bloch vectors corresponding to projections onto orthogonal states sum up to the zero vector, the corresponding probabilities assigned by a \(HV\) state sum up to 1, as it should be. Thus, the set of \(HV\) states corresponding to vertices of the dual polytope is sufficient for a preparation-universal \(HV\) model. Note that this model can in general be indeterministic. In such a case, each indeterministic \(HV\) state can be further reduced into at most \(N - 2\) deterministic \(HV\) states, according to (3).

The reason for \(N - 2\), and not \(N + 1\), states stems from the observation that a vertex of the dual polytope saturates at least three of the inequalities defining the polytope (at least three facets have to meet at each vertex), i.e., the corresponding probability is 1 or 0, and reduces the number of required deterministic \(HV\) states. Finally, the total number of \(HV\) states required for an indeterministic model is \(L \leq F\), and for a deterministic model is \(L \leq (N - 2)F\), where \(F\) is the number of vertices of the dual polytope or, equivalently, the number of
facets of the measurement polytope. A convex polytope with $2N$ vertices (in three-dimensional space) can have $N + 2 \leq F \leq 4(N - 1)$ facets [13], which implies that indeterministic HV models require at most a number of HV states that is linear in $N$, and deterministic ones require quadratic number of HV states.

Using the dual polytope approach, we generalize Spekkens’ model [6], originally formulated to explain the measurement results on the eigenstates of the three complementary directions, to the preparation-universal model. For these directions, the measurement polytope is an octahedron, see Fig. 1(a). The dual polytope is a cube, whose interior forms the whole space of HV states, with the vertices being the deterministic states. Another interesting example is illustrated in Fig. 1(b).

The dual polytope approach can be applied to arbitrary preparation vectors. However, efficient simulations are only expected for highly symmetric polytopes. For this reason, we move to more complicated Platonic solids and general symmetry considerations.

Consider a set of measurement directions $\pm m_1, \ldots, \pm m_N$, which is generated by a group; e.g., an octahedron and a cube can be generated via the chiral octahedral group $O$ with 24 rotations. Generally, if $G$ is a symmetry of the measurement polytope, $M$, it is also a symmetry of its dual, $D_M$: i.e., the dual polytope can also be generated by $G$. The group action permutes the vectors $\pm m_i$ as well as vertices of the dual polytope. Since the last are related to the HV states, we can define the permutation representation of the group in the HV space, $D_P(G)$. The HV state, $h(y')$, corresponding to a vertex of a dual polytope, $y' = gy$, which is generated by $g \in G$ acting on an initial vertex, $y$, can be found using the group representation:

$$h(gy) = D_P(g)h(y). \quad (7)$$

Decomposing $h(y)$ into deterministic HV states brings (7) to the form $h(gy) = \sum_{\alpha} \alpha h(D_P(g)\alpha)$. Therefore, the set of deterministic HV states required for the preparation-universal model is the union of a number of group orbits $\{D_P(g)\alpha | g \in G\}$. Because of the symmetries involved, the minimal number of HV states cannot be smaller than the number of elements in the smallest orbit.

Let us consider two other Platonic solids, the icosahedron and the dodecahedron [17]. Both of them possess the same symmetry, the chiral icosahedral group $I_d$, with 60 rotations. Consider the icosahedron as the measurement polytope, $N = 6$. Its dual, the dodecahedron, has 20 vertices corresponding to indeterministic HV states that can be further reduced to deterministic HV states. The total number of possible deterministic HV states is $2^6 = 64$ in this case. We have found four different orbits of action of $I_d$ with 12, 12, 20, 20 different elements, respectively. Only one orbit, with 20 elements, gives deterministic states for universal simulation. For $N = 10$ measurement settings, the dodecahedron is the measurement polytope. Its dual, the icosahedron, has 12 vertices. The total number of possible deterministic HV states is $2^{10} = 1024$, which is partitioned into 24 different orbits: 2 with 12 elements, 8 with 20, and 14 with 60 elements. The two lowest orbits are suitable for the universal model. Thus, the minimal deterministic model, among all HV models obtained through the dual polytope construction, requires only 24 HV states, twice the number of vertices of the dual polytope.

The presentation so far was limited to qubits. However, a similar line of reasoning applies to any $d$-level quantum system. In the general case, Pauli operators have to be replaced by generalized Gell-Mann operators, $\lambda_i$, which naturally leads to the generalized, $D \equiv d^2 - 1$ dimensional, Bloch representation. An arbitrary quantum state, $\hat{\rho} = \frac{1}{d}[1 + (d - 1) \sum_{i=1}^D x_i \lambda_i]$, is now represented by a generalized Bloch vector, $x$, with components $x_i = \text{Tr}(\hat{\rho} \lambda_i)$. We normalize the Gell-Mann operators as $\text{Tr}(\lambda_i \lambda_j) = \frac{d}{2} \delta_{ij}$, such that pure quantum states are represented by normalized generalized Bloch vectors. Contrary to the qubit case, not every unit vector corresponds to a physical state. The probability of an outcome associated with a projector on a state represented by $\mathbf{m}_n$, in a measurement on a state represented by $x$, is $p_n(x) = \frac{1}{d}[1 + (d - 1) (\mathbf{m}_n \mathbf{x})]$. The requirement of positive probabilities reveals that, e.g., the vector $x = -\mathbf{m}_n$ does not represent a physical state.
In analogy to the dual polytope, for a set of $dN$ preparation vectors, representing $N$ $d$-valued observables, we introduce a convex polytope the interior of which includes all vectors $y$ leading to physically allowed probabilities $p_n(y) \in [0,1]$: \[ \mathcal{P}_M = \{ y \in \mathbb{R}^D | -\frac{1}{d-1} \leq m_n y \leq 1, n = 1, ..., dN \}. \] (8)

Among others, this polytope contains all the vectors of quantum states. The generalized Bloch vectors corresponding to a complete set of orthogonal quantum states sum up to the zero vector, implying the probabilities assigned by a HV state for different outcomes of any measurement sum up to 1, as it should be. Again, the vectors of quantum states can be expressed as a convex combination of vertices of $\mathcal{P}_M$, and their number gives the upper bound on the amount of HV states sufficient for preparation-universal simulation. The polytope $\mathcal{P}_M$ is specified by $q = 2dN$ linear inequalities, two inequalities for each vector $m_n$, and its maximal number of vertices is given by $L \leq \left( \frac{q-1}{q-D} \right) + \left( \frac{q-1}{q-D} \right)$, where $\delta \equiv \left\lfloor (D + 1)/2 \right\rfloor$, $\delta' \equiv \left\lfloor (D + 2)/2 \right\rfloor$, and $\lfloor x \rfloor$ is the integer part of $x$ [13]. In the special case of a qubit, the dual polytope is defined by $2N$, and not $4N$, inequalities because the two bounds of Eq. (6) are the same for the vectors $\pm m_n$. Since the binomial coefficient $\binom{q}{a}$ increases with $a$, $L \leq 2^q (q-D)$. Using $\binom{q}{a} = \binom{q}{a}$, we have $L \leq 2^q (q-D)$, and since $\binom{q}{a} \leq a^b/b!$, the maximal number of vertices is polynomial in $N$, $L \sim (2dN - \delta)^{D-\delta}$. The related HV states can in general be indeterministic, and each of them can be decomposed to $O(N)$ deterministic HV states, using decomposition [9] in the $dN$ dimensional space $\Lambda$. Therefore, for any system, the number of (in)deterministic HV states required for a preparation-universal simulation is polynomial in $N$.

In the limit of infinitely many measurements, our method gives (preparation and measurement) universal models with the minimal number of HV states. As proved by Montina, in this limit the optimal model requires $2(d-1)$ real parameters to describe the HV states [10]. We show that for an infinite number of settings the set of universal HV states converges to the set of pure quantum states, which is known to be parameterized by $2(d-1)$ real numbers. First, consider a finite set of projectors $\Pi_n$ with $n = 1, ..., dN$, and the corresponding polytope [3] in the Hilbert-Schmidt space of Hermitian operators with unit trace. The operators of its vertices, $\hat{y}_l$, correspond to the HV states, i.e., for all $n$, $\text{Tr}(\hat{y}_l \Pi_n)$ gives the probability that is assigned by the HV state, of the outcome associated with projector $\Pi_n$. For other projectors, not within the set of $dN$, the trace does not have to represent a probability and therefore the set of operators $\hat{y}_l$ is larger than the set of quantum states [15]. However, in the limit of infinitely many measurements, $\text{Tr}(\hat{y}_l \Pi_n) \in [0,1]$ for all possible projectors; therefore, the eigenvalues of $\hat{y}_l$’s lie within the $[0,1]$ interval. Since $\text{Tr}(\hat{y}_l) = 1$, the operators $\hat{y}_l$ are just quantum states and the HV states corresponding to pure quantum states are universal. Their number scales linearly with $N$, because $N$ measurements correspond to $dN$ projectors and each of them represents one HV state (and also one pure quantum state).

Regarding the polytope $\mathcal{P}_M$ in the space of Hermitian operators allows for an easy generalization of our approach to POVM measurements. POVM elements, $E_n$, are positive operators being vertices of a measurement polytope. The polytope $\mathcal{P}_M$ includes all the unit-trace operators $\hat{y}$ for which $\text{Tr}(\hat{y} E_n) \in [0,1]$. Since for all quantum states $\text{Tr}(\hat{y} E_n) \in [0,1]$, the polytope $\mathcal{P}_M$ contains all of them and, as before, its vertices define HV states.

For a $d$-level system the KS argument disqualifies non-contextual HV theories [2], and one might wonder how contextuality enters our models. Consider the KS argument of Peres [14]. It involves 33 different vectors in $\mathbb{R}^3$, which belong to 16 different orthogonal triads. Non-contextuality requires a value associated with a single vector to be the same irrespectively of other vectors in the triad. In the present models, the results of 16 different measurements are described by HV states with $3 \cdot 16 = 48$ components; i.e., a value assigned to the same vector can depend on the other vectors in the triad.

In conclusion, we proved that a preparation-universal HV model of the results of $N$ quantum measurements requires at most a number of HV states which is polynomial in $N$. In the limit of infinitely many measurements, our method gives optimal preparation- and measurement-universal HV models, with the minimal number of real parameters describing the HV states. There is no HV model that would require less HV states than the model in which every quantum state is associated with a HV state [10]. Furthermore, since there are infinitely many measurements that can be performed on a quantum system, its HV description requires infinitely many HV states. This “ontological baggage” [8] can be seen as an argument against the HV approach because it is extremely resource demanding already for a single qubit.

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[15] The Carathéodory’s theorem states that a point, \( x \), in a convex polytope in \( \mathbb{R}^n \) can be written as a convex combination of \( n + 1 \) vertices.
[16] In the special case of measurement settings within a plane, we consider the dual polygon lying in that plane.
[17] Similar analysis applies to cube and octahedron.
[18] E.g., if the preparation vector of a qubit involves projectors on \( |\pm\rangle \) and \( |x\rangle \), it is valid to consider \( \hat{y}_t = \frac{1}{2} \mathbb{1} + \hat{\sigma}_x + \hat{\sigma}_z \), which is not a quantum state.