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Learning optimal quantum models is NP-hard

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Physical modeling translates measured data into a physical model. Physical modeling is a major objective in physics and is generally regarded as a creative process. How good are computers at solving this task? Here we show that in the absence of physical heuristics, the inference of optimal quantum models cannot be computed efficiently (unless $P = NP$). This result illuminates rigorous limits to the extent to which computers can be used to further our understanding of nature.

A characterization of a physical experiment is always at least two-fold. On the one hand, we have a description

$$\mathcal{S} = (\text{description of the state})$$

of the state of the physical system. For instance, \mathcal{S} can contain a few paragraphs of text with detailed instructions for preparing that state experimentally in the lab, or for finding it in nature.

The second part of the characterization of an experiment is the description of the measurement that is performed. As for the state, the measurement may be described in terms of a short text,

$$\mathcal{M} = (\text{description of the measurement}).$$

\mathcal{M} may be a complete manual for constructing the measurement device we use.

Both \mathcal{M} and \mathcal{S} can specify *temporal* and *spatial* information, e.g., the desired state is the state resulting from a particular initial state after letting it evolve for $1\mu\text{s}$. Every experimental paper must provide \mathcal{M} and \mathcal{S} .

Performing the measurement \mathcal{M} results in a *measurement outcome*. We denote by Z the number of different measurement outcomes. Each of the outcomes may again be characterized in terms of a few paragraphs of text

$$\mathcal{O}_z = (\text{description of } z\text{th measurement outcome})$$

for all $z \in [Z] := \{1, \dots, Z\}$. Here we assume without loss of generality that the description \mathcal{O}_z also specifies \mathcal{M} , i.e., it both fully specifies the measurement device and the way it signals ‘*outcome z has been measured*’ to the observer.

Oftentimes we do not only consider a single state \mathcal{S} and a single measurement $(\mathcal{O}_z)_{z \in [Z]}$ but X states $(\mathcal{S}_x)_{x \in [X]}$ and Y measurements $(\mathcal{O}_{yz})_{z \in [Z]}$ ($y \in [Y]$). For instance, we could be interested in measuring the spin of an electron in different directions and at different times. Repeatedly measuring the state \mathcal{S}_x with the measurement \mathcal{M}_y we are able to collect *empirical frequency distributions* $(f_{xyz})_{z=1}^Z$ for that particular sequence of measurements. I.e., $f_{xyz} = \sharp\{z|xy\}/N_{xy}$ where N_{xy} denotes the number of times we measure \mathcal{S}_x with \mathcal{M}_y and where

$\sharp\{z|xy\}$ denotes the number of times we see outcome \mathcal{O}_{yz} during these runs of the experiment.

To describe the experiment quantum mechanically we need to translate the descriptions \mathcal{S}_x and \mathcal{O}_{yz} into quantum states ρ_x and measurement operators E_{yz} . This corresponds to the task of modeling. The assignment of matrices to \mathcal{S}_x and \mathcal{O}_{yz} must be such that the quantum mechanical predictions are compatible with the previously measured data f_{xyz} . By Born’s rule, $\text{tr}(\rho_x E_{yz})$ is the probability for measuring outcome z if we measure state \mathcal{S}_x with the measurement \mathcal{M}_y . Hence, achieving compatibility between the theoretical model ρ_x, E_{yz} on the one hand and the experimental description $\mathcal{S}_x, \mathcal{O}_{yz}$ on the other hand requires to searching states and measurements satisfying $\text{tr}(\rho_x E_{yz}) \approx f_{xyz}$ for all $(x, y, z) \in \Omega$. Here, $\Omega \subseteq [X] \times [Y] \times [Z]$ marks the particular combinations (x, y, z) that we have measured experimentally. Combinations in the complement $(x, y, z) \in \Omega^c$ are unknown. A common pitfall to avoid is *overfitting*, that is, finding an excessively complicated model that perfectly fits the data but has no predictive power over future observations. To avoid overfitting we need to search for the lowest-dimensional model satisfying $\text{tr}(\rho_x E_{yz}) \approx f_{xyz}$. In fact, if we placed no restriction on the dimension, then we could fit every dataset exactly with a *finite-dimensional* quantum model that does not allow for the prediction of future measurement outcomes. For instance, we could fit the measured data with an X -dimensional model where $\rho_x = |x\rangle\langle x|$ and $E_{yz} = \sum_{x=1}^X f_{xyz}|x\rangle\langle x|$. Indeed, $\text{tr}(\rho_x E_{yz}) = f_{xyz}$. On the other hand, if a subsystem structure (e.g., two independent parties Alice and Bob) is imposed then there are circumstances where datasets cannot be modeled by finite-dimensional quantum models [1, 2].

In the remainder we are going to assume that the empirical frequencies f_{xyz} are equal to the probabilities p_{xyz} for measuring outcome \mathcal{O}_{yz} given that we prepared \mathcal{S}_x and measured \mathcal{M}_y . This condition is met if we can measure states \mathcal{S}_x with measurements \mathcal{M}_y an unbounded number of times ($N_{xy} \rightarrow \infty$). We will see that inference is *NP-hard* even in this noiseless setting where we

want to solve

$$\begin{aligned} & \text{minimize } d \\ & \text{such that } \exists d\text{-dimensional states and measurements} \\ & \text{satisfying } p_{xyz} = \text{tr}(\rho_x E_{yz}) \quad \forall (x, y, z) \in \Omega. \end{aligned} \quad (1)$$

We call problem (1) *MinDim*; it describes the task of *learning effective quantum models* from experimental data. Our result that *MinDim* is *NP-hard* implies that computers are not capable of computing optimal quantum models describing general experimental observations (unless $P = NP$).

NP-hardness is a term from *computational complexity theory* which aims at classifying problems according to their complexity. The relevant complexity measure depends on the particular application. Here we focus on *time complexity* which measures the time it takes to solve a problem on a computer (deterministic Turing machine). A particularly important family of problems are *decision problems*. These are problems whose solution is either *yes* or *no*. 3-coloring of graphs is a famous example. In 3-coloring (*3col*) we are given a graph with vertices specified by a vertex set V and with edges specified by an edge set E . Our task is to decide whether or not it is possible to assign colours *red*, *green* or *blue* to vertices $v \in V$ in such a way that vertices v, v' are colored differently whenever the edge (v, v') with endpoints v, v' is an element of E . In this example, the specification of V and E forms the *problem instance* and the criterion for the solution *yes* (i.e., ‘yes, this graph is 3-colorable’) is the so called *acceptance condition*. A decision problem is specified by an acceptance condition and by a set of problem instances.

The complexity classes P and NP have been introduced to classify problems according to their complexity. The complexity class P is the set of all decision problems whose complexity is a polynomial in the size of the problem instances (e.g., the number of vertices in case of *3col*). The class NP is the set of problems with the following property. Every *yes*-instance admits a proof that can be checked in polynomial time. For example in case of *3col*, we can prove that a graph is 3-colorable by providing an explicit 3-coloring of that graph; the correctness of that coloring can be verified by checking that for all $(v, v') \in E$, the vertices v and v' are colored differently.

Intuitively, a problem A is clearly harder to solve than a problem B if any polynomial-time algorithm for A can be used to solve B in polynomial time (we might use the algorithm for A as a subroutine in another algorithm to solve B). This intuition is rigorously captured in the notion of reductions. We say that problem B is *reducible* to A if there exists an algorithm \mathcal{A} (polynomial-time) that maps problem instances i for B to problem instances

$\mathcal{A}(i)$ for A in such a way that

$$i \text{ ‘yes’ for } B \Leftrightarrow \mathcal{A}(i) \text{ ‘yes’ for } A.$$

Therefore, if there exists a polynomial-time algorithm to solve A then this algorithm induces via \mathcal{A} a polynomial time algorithm to solve B . A problem A is *NP-hard* if all problems $C \in NP$ are reducible to A . For example, *3col* is *NP-hard* [3].

A natural decision version of *MinDim* is the problem *Dim-d*.

Dim-d. Instance: $X, Y, Z \in \mathbb{N}$, $\Omega \subseteq [X] \times [Y] \times [Z]$ and scalars $(p_{xyz})_{x,y,z \in \Omega}$. *Acceptance condition:* there exist d -dimensional states ρ_x and measurements $(E_{yz})_{z \in [Z]}$ such that $p_{x,y,z} = \text{tr}(\rho_x E_{yz})$ for all $(x, y, z) \in \Omega$.

We note that *Dim-d* outputs *yes* if and only if the optimal solution d_{MinDim} of *MinDim* satisfies $d_{\text{MinDim}} \leq d$. Hence, *MinDim* is *NP-hard* if *Dim-3* is *NP-hard*. In this work, we prove the latter by reduction from *3col*. Thus, we are arriving at our main result, Theorem 1.

Theorem 1. *MinDim is NP-hard.*

Every experiment can be described in terms of $(\mathcal{S}_x)_x$ and $(\mathcal{O}_{yz})_{yz}$. Therefore, problem (1) does not make any assumptions about the underlying quantum model. Often, however, we accept some side information about the physical system we wish to analyze. A common postulate is that we measure a global state with local measurements [4–7]. In this setting we want to solve the following modification of *MinDim*.

$$\begin{aligned} & \text{minimize } d \\ & \text{such that } \exists \text{ a } d^2\text{-dimensional state } \rho \text{ and } d\text{-dimensional} \\ & \text{measurements } (E_{yz})_z \text{ and } (F_{yz})_z \text{ satisfying} \\ & p_{yzy'z'} = \text{tr}(\rho E_{yz} \otimes F_{y'z'}) \quad \forall (yzy'z') \in \Omega \end{aligned} \quad (2)$$

(for some $\Omega \subseteq [Y] \times [Z] \times [Y'] \times [Z']$). We are referring to problem (2) in terms of *MinDim*^(AB); the label (AB) references two parties, usually called Alice and Bob. Here we prove *NP-hardness* of *MinDim*^(AB) by showing that the natural decision problem *Dim-3*^(AB) (see the supplementary material) of *MinDim*^(AB) is *NP-hard*.

Theorem 2. *MinDim*^(AB) *is NP-hard.*

Theorems 1 and 2 assume that the measurement probabilities p_{xyz} and $p_{yzy'z'}$ are known exactly. Hence, Theorem 1 and 2 do not allow to draw rigorous conclusions about situations where p_{xyz} are only known approximately. When does a physical theory qualify to be a good physical theory? Answers provided are sometimes vague. However, there is a consensus that *predictive power* is a necessary criterion a good physical theory needs to satisfy. This criterion is satisfied if models drawn from that

theory (e.g., quantum theory) allow for the prediction of future measurement outcomes, i.e., estimates of probabilities p_{xyz} associated to pairings $(\mathcal{S}_x, \mathcal{O}_{yz})$ that have not been measured yet (i.e., $(x, y, z) \notin \Omega$ in problem *MinDim*). For example, if x enumerates the states of a system at different times, then we would like to be able to predict future measurement outcomes. Therefore, considering Theorem 1 in the scenario where all probabilities p_{xyz} were measured beforehand (i.e., $\Omega = [X] \times [Y] \times [Z]$) would not be very sensible because there would not be anything left to predict. Results of hardness in this setting are, however, of interest in mathematical optimization where people study the optimal runtime of semidefinite program formulations of linear optimization problems [8–12].

Surprisingly, problem *MinDim* has only been studied sporadically [6, 13–20, 20, 21]. Related to *MinDim* is the problem of estimating quantum processes in a way that is robust to prepare and measure errors [22–27]. Moreover, *MinDim* realizes a non-commutative version of topic models which one may want to call *quantum topic models* [28]. In relation to inference of dynamics, previous seminal work [29] showed that the *identification of dynamical laws* is *NP*-hard. In contrast, our work does not assume Markovianity. Non-Markovian dynamics has been intensively investigated in the past years; see, e.g., [30, 31]. Theorem 5.6 of [10] would be sufficient to prove *NP*-hardness of *MinDim* if we were given an a priori promise that the considered dataset $(p_{xyz})_{xyz}$ was generated by measuring pure states with rank-1 measurements. Distinguishing these datasets from general datasets is an interesting open problem.

In quantum state tomography we aim at inferring a quantum state ρ after having postulated the Hilbert space dimension and the measurement representations E_{yz} . Research on quantum state tomography is more mature than research on *MinDim*: efficient algorithms are known and it is possible to report confidence regions in situations where ρ has been measured a finite number of times [32, 33]. Model selection [34–36] has been applied widely to overcome assumptions underlying state tomography. It is an interesting open problem to analyze these model selection methods from the perspective of computational complexity theory.

Sketch of the proof. We prove Theorem 1 by showing that *Dim-3* is *NP*-hard. Figure 1 sketches the strategy of our proof. We construct a sequence of reductions whose composition reduces *3col* to *Dim-3*. This suffices to prove Theorem 1 because *3col* is known to be *NP*-hard [3]. Analogously, we prove Theorem 2 by showing that the associated decision problem *Dim-3*^(AB) is *NP*-hard.

Thus, to prove Theorem 1, we need to find a polynomial-time algorithm \mathcal{A} that maps instances for *3col* to instances of *Dim-3* such that an instance i for *3col* is a *yes*-instance for *3col* if and only if $\mathcal{A}(i)$ is a

yes-instance for *Dim-3*. As suggested by figure 1, the reduction \mathcal{A} is the composition of several partial reductions, i.e., $\mathcal{A} = \mathcal{A}_3 \circ \mathcal{A}_2 \circ \mathcal{A}_1$. Each of the parts \mathcal{A}_1 , \mathcal{A}_2 , \mathcal{A}_3 are defined in the remainder of this section. The reduction \mathcal{A}_0 from any problem in *NP* to *3col* is introduced in [3]. Consequently, reductions $\mathcal{A} \circ \mathcal{A}_0$ reduce any problem in *NP* to *Dim-3*.

In the supplementary material we provide the analysis of the algorithms \mathcal{A}_j and the formal proof of Theorem 1. Similarly, to prove Theorem 2 we provide a reduction $\mathcal{A}' = \mathcal{A}'_3 \circ \mathcal{A}_2 \circ \mathcal{A}_1$ from *3col* to *Dim-3*^(AB). Here, the sub-reductions \mathcal{A}_1 and \mathcal{A}_2 are identical to the sub-reductions used in the proof of Theorem 1. Only the last sub-reduction \mathcal{A}_3 requires modification. That modification \mathcal{A}'_3 and its discussion are provided in the supplementary material.

In the remainder we provide a short sketch of the individual parts of the proof of Theorem 1. Following [37], we say a matrix $A \in \mathbb{C}^{|V| \times |V|}$ fits a graph $G = (V, E)$ if

- $A_{jj} = 1$ for all $j \in V$, and if
- $A_{ij} = 0$ for all $(i, j) \in E$.

Using a key Theorem from [37] we can show in Lemma 5 (\Leftrightarrow reduction \mathcal{A}_1) of the supplementary material that a graph G is 3-colorable if and only if a graph $\Delta(G')$ (a transformation of G) can be fitted by a Gram matrix A with matrix rank ≤ 3 .

Subsequently, we show in Lemma 6 (\Leftrightarrow reduction \mathcal{A}_2) that this Gram matrix A exists if and only if there exist 3-dimensional vectors ψ_j such that the matrix with elements $p_{ij} := |\bar{\psi}_i^T \psi_j|^2$ fits $\Delta(G')$.

The transformation $\Delta(G')$ of G is chosen such that these vectors ψ_j exist if and only if there exists a 3-dimensional quantum model with the following property: the matrix $(\text{tr}(\rho_x E_{yz}))_{x,yz}$ fits $\Delta(G')$. This is observation forms the content of Lemma 7 (\Leftrightarrow reduction \mathcal{A}_3). Checking whether or not there exists a 3-dimensional quantum model fitting $\Delta(G')$ is a special instance of *Dim-3*.

We thus conclude that a polynomial-time algorithm for *Dim-3* can be used for checking (in polynomial time) whether or not a graph G is 3-colorable. The proof of Theorem 2 proceeds along the same lines. We only need to modify the reduction \mathcal{A}_3 .

Conclusions. We have shown that optimal quantum models cannot be computed efficiently from measured data. We proved this claim in both the natural 1-party (cf. Theorem 1) and the natural 2-party setting (cf. Theorem 2). We proved *NP*-hardness by reducing 3-coloring to the inference of quantum models.

What other questions remain in this field? In both Theorem 1 and Theorem 2 we search for a quantum model which reproduces the measured probabilities exactly. Does the hardness result extend to situations where we are satisfied with only approximating the

measured probabilities? And which classes of data $(p_{xyz})_{(xyz) \in \Omega}$ admit efficient inference? In regard of the latter question, it appears important to illuminate the *tradeoff* between

- the relevance of the class of considered datasets $\{(p_{xyz})_{(xyz) \in \Omega}\}$ and
- the computational hardness of inference associated to those datasets.

The hardness of the classical analog of *MinDim* turns out to be easier to prove as it directly reduces from the problem of computing the so called nonnegative rank which is known to be *NP*-hard [38].

Added Note. After we uploaded this paper to the arXiv, Yaroslav Shitov uploaded the independent seminal preprint [39]. Yaroslav Shitov’s paper proves *NP*-hardness of the real psd rank (i.e., the psd factors have real matrix entries). If Yaroslav Shitov’s proof can be generalized to the complex setting then Theorem 1 can be derived as simple corollary; see Lemma 17 in [40].

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- [1] Ravishankar Ramanathan, Jan Tuziemski, Michał Horodecki, and Paweł Horodecki. *arXiv:1410.0947*, 2014.
 - [2] Jamie Sikora, Antonios Varvitsiotis, and Zhaohui Wei. *arXiv:1507.00213*, 2015.
 - [3] Michael R Garey, David S Johnson, and Larry Stockmeyer. *Theoretical computer science*, 1(3):237–267, 1976.
 - [4] Sandu Popescu and Daniel Rohrlich. *Foundations of Physics*, 24(3):379–385, 1994.
 - [5] Miguel Navascués, Stefano Pironio, and Antonio Acín. *New Journal of Physics*, 10(7):073013, 2008.
 - [6] Miguel Navascués, Adrien Felix, Mateus Araujo, and Tamas Vertesi. *arXiv:1507.07521*, 2015.
 - [7] Roger Colbeck and Renato Renner. *Nature Physics*, 8(6):450–453, 2012.
 - [8] Samuel Fiorini, Serge Massar, Sebastian Pokutta, Hans Raj Tiwary, and Ronald de Wolf. pages 95–106. ACM, 2012.
 - [9] Joao Gouveia, Pablo A Parrilo, and Rekha R Thomas. *Mathematics of Operations Research*, 38(2):248–264, 2013.
 - [10] Hamza Fawzi, João Gouveia, Pablo A Parrilo, Richard Z Robinson, and Rekha R Thomas. *arXiv:1407.4095*, 2014.
 - [11] Zhengfeng Ji. *arXiv:1310.3794*, 2013.
 - [12] Sabine Burgdorf, Monique Laurent, and Teresa Piovesan. *arXiv:1502.02842*, 2015.
 - [13] Cyril Stark. *Physical Review A*, 89(5):052109, 2014.
 - [14] Denis Rosset, Raphael Ferretti-Schöbitz, Jean-Daniel Bancal, Nicolas Gisin, and Yeong-Cherng Liang. *Physical Review A*, 86(6):062325, 2012.
 - [15] Cyril J Stark and Aram W Harrow. *arXiv:1412.7437*, 2014.
 - [16] Rodrigo Gallego, Nicolas Brunner, Christopher Hadley, and Antonio Acín. *Physical review letters*, 105(23):230501, 2010.
 - [17] Nicholas Harrigan, Terry Rudolph, and Scott Aaronson. *arXiv:0709.1149*, 2007.
 - [18] Stephanie Wehner, Matthias Christandl, and Andrew C Doherty. *Physical Review A*, 78(6):062112, 2008.
 - [19] Cyril Stark. *arXiv:1209.6499*, 2012.
 - [20] Christopher Jackson and SJ van Enk. *arXiv:1508.05633*, 2015.
 - [21] Shelby Kimmel and Yi-Kai Liu. *arXiv:1510.08887*, 2015.
 - [22] S.T. Merkel, J.M. Gambetta, J.A. Smolin, S. Poletto, A.D. Córcoles, B.R. Johnson, C.A. Ryan, and M. Steffen. *arXiv:1211.0322*, 2012.
 - [23] R. Blume-Kohout, J.K. Gamble, E. Nielsen, J. Mizrahi, J.D. Sterk, and P. Maunz. *arXiv:1310.4492*, 2013.
 - [24] Shelby Kimmel, Marcus P da Silva, Colm A Ryan, Blake R Johnson, and Thomas Ohki. *Physical Review X*, 4(1):011050, 2014.
 - [25] Shelby Kimmel, Guang Hao Low, and Theodore J Yoder. *arXiv:1502.02677*, 2015.
 - [26] Arnaud C Dugas, Joel Wallman, and Joseph Emerson. *arXiv:1508.06312*, 2015.
 - [27] Alex Monras and Andreas Winter. *arXiv:1412.3634*, 2014.
 - [28] Cyril Stark. *arXiv:1601.06035*, 2016.
 - [29] Toby S Cubitt, Jens Eisert, and Michael M Wolf. *Physical review letters*, 108(12):120503, 2012.
 - [30] Ángel Rivas, Susana F Huelga, and Martin B Plenio. *Reports on Progress in Physics*, 77(9):094001, 2014.
 - [31] Juan P Dehollain, Juha T Muhonen, Robin Blume-Kohout, Kenneth M Rudinger, John King Gamble, Erik Nielsen, et al. *arXiv:1606.02856*, 2016.
 - [32] Philippe Faist and Renato Renner. *arXiv preprint arXiv:1509.06763*, 2015.
 - [33] Robin Blume-Kohout. *arXiv preprint arXiv:1202.5270*, 2012.
 - [34] Mădălin Guță, Theodore Kypraios, and Ian Dryden. *New Journal of Physics*, 14(10):105002, 2012.
 - [35] SJ Van Enk and Robin Blume-Kohout. *New Journal of Physics*, 15(2):025024, 2013.
 - [36] Christopher Ferrie. *New Journal of Physics*, 16(9):093035, 2014.
 - [37] René Peeters. *Combinatorica*, 16(3):417–431, 1996.
 - [38] Stephen A Vavasis. *SIAM Journal on Optimization*, 20(3):1364–1377, 2009.
 - [39] Yaroslav Shitov. *arXiv:1606.09065*, 2016.
 - [40] Troy Lee, Zhaohui Wei, and Ronald de Wolf. *arXiv:1407.4308*, 2014.

Figures

FIG. 1: Successive reduction from problems in *NP* to *Dim-3*.

