Learning optimal quantum models is NP-hard

Citation: Stark, Cyril J. et al. "Learning optimal quantum models is NP-hard. " Physical Review A 97, 2 (February 2018): 020103(R) © 2018 American Physical Society

As Published: http://dx.doi.org/10.1103/PhysRevA.97.020103

Publisher: American Physical Society

Persistent URL: http://hdl.handle.net/1721.1/114464

Version: Final published version: final published article, as it appeared in a journal, conference proceedings, or other formally published context

Rapid Communications

Learning optimal quantum models is NP-hard

Cyril J. Stark
Center for Theoretical Physics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139-4307, USA

(Received 19 August 2016; published 8 February 2018)

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.

DOI: 10.1103/PhysRevA.97.020103

A characterization of a physical experiment is always at least twofold. 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 laboratory, 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 μs. 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 $z \in [Z] := \{1, \ldots, Z\}$. 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, that is, $f_{xyz} = \sharp\{z|xy\}/N_{xy}$, 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, $\mathrm{tr}(\rho_x E_{yz})$ 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 searching for states and measurements satisfying $\mathrm{tr}(\rho_x E_{yz}) \approx f_{xyz}$ 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 $\mathrm{tr}(\rho_x E_{yz}) \approx f_{xyz}$. In fact, if we placed no restriction on the dimension, then we could fit every data set 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, $\mathrm{tr}(\rho_x E_{yz}) = f_{xyz}$. On the other hand, if a subsystem structure (e.g., two independent parties Alice and Bob) is imposed, then there are circumstances where data sets 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 $(N_{xy} \to \infty)$. We will see that inference is NP-hard even in this noiseless setting where we want to solve

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

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*. The 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 colors *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 the 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 $p_{x;yz} = \mathrm{tr}(\rho_x E_{yz})$ 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 $d_{\mathrm{MinDim}} \leqslant d$. Hence, MinDim is NP-hard if Dim-3 is NP-hard. In this Rapid Communication, 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 $(\mathcal{O})_{yz}$. 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,

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

(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 Supplemental Material [8]) 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, Theorems 1 and 2 do not allow one 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 [9–13].

Surprisingly, problem MinDim has only been studied sporadically [6,14–22]. Related to MinDim is the problem of estimating quantum processes in a way that is robust to prepare and measure errors [23–28]. Moreover, MinDim realizes a noncommutative version of topic models which one may want to call *quantum topic models* [29]. In relation to inference of dynamics, previous seminal work [30] showed that the *identification of dynamical laws* is NP-hard. In contrast, our work does not assume Markoviantity. Non-Markovian dynamics has been intensively investigated in the past years; see, e.g., Refs. [31,32]. Theorem 5.6 of Ref. [11] would be sufficient to prove NP-hardness of MinDim if we were given an *a priori* promise that the considered data set $(p_{xyz})_{xyz}$ was

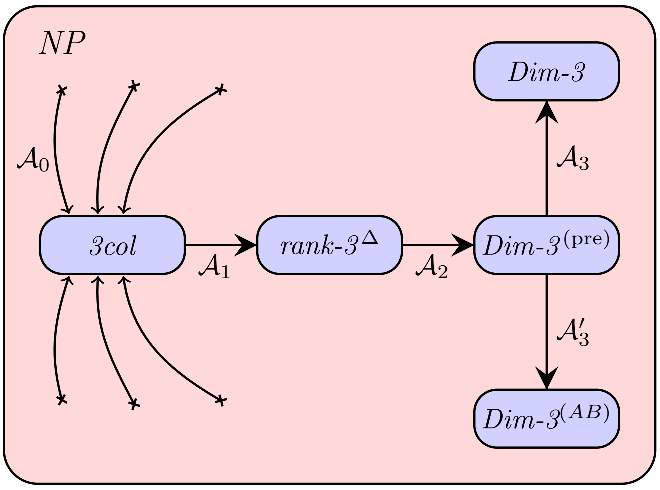

FIG. 1. Successive reduction from problems in NP to Dim-3.

generated by measuring pure states with rank-1 measurements. Distinguishing these data sets from general data sets 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 [33,34]. Model selection [35–37] 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 Fig. 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 Ref. [3]. Consequently, reductions $\mathcal{A} \circ \mathcal{A}_0$ reduce any problem in NP to Dim-3.

In the Supplemental Material [8] 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 subreductions $\mathcal{A}_1$ and $\mathcal{A}_2$ are identical to the subreductions used in the proof of Theorem 1. Only the last subreduction $\mathcal{A}_3$ requires modification. That modification $\mathcal{A}_3'$ and its discussion are provided in the Supplemental Material [8].

In the remainder we provide a short sketch of the individual parts of the proof of Theorem 1. Following Ref. [38], we say a matrix $A \in \mathbb{C}^{|V|\times|V|}$ fits a graph $G = (V,E)$ if (i) $A_{jj} = 1$ for all $j \in V$, and if (ii) $A_{ij} = 0$ for all $(i,j) \in E$.

Using a key theorem from Ref. [38] we can show in Lemma 5 ($\leftrightarrow$ reduction $\mathcal{A}_1$) of the Supplemental Material [8] 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 $\leqslant 3$.

Subsequently, we show in Lemma 6 ($\leftrightarrow$ reduction $\mathcal{A}_2$) that this Gram matrix A exists if and only if there exist three-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 three-dimensional quantum model with the following property: The matrix $[\mathrm{tr}(\rho_x E_{yz})]_{x;yz}$ fits $\Delta(G')$. This is observation forms the content of Lemma 7 ($\leftrightarrow$ reduction $\mathcal{A}_3$). Checking whether or not there exists a three-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 Theorems 1 and 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 (i) the relevance of the class of considered data sets $\{(p_{xyz})_{(xyz)\in\Omega}\}$ and (ii) the computational hardness of inference associated to those data sets.

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 non-negative rank which is known to be NP-hard [39].

Note added. Recently, we became aware of Shitov's independent seminal work [40]. Shitov's paper proves NP-hardness of the real psd rank (i.e., the psd factors have real matrix entries). If Shitov's proof can be generalized to the complex setting, then Theorem 1 can be derived as a simple corollary; see Lemma 17 in Ref. [41].

Acknowledgments. I would like to thank Aram Harrow, Robin Kothari, Lior Eldar, Pablo Parrilo, Jonathan Kelner, Ankur Moitra, Lídia del Rio, Adam Sawicki, and Antonios Varvitsiotis for interesting discussions. In particular I would like to thank Matt Coudron for fruitful discussions and for pointing out Ref. [38]. This work is supported by the ARO grant Contract No. W911NF-12-0486. This work is preprint MIT-CTP/4719.

[1] R. Ramanathan, J. Tuziemski, M. Horodecki, and P. Horodecki, Phys. Rev. Lett. **117**, 050401 (2016).
[2] J. Sikora, A. Varvitsiotis, and Z. Wei, Phys. Rev. Lett. **117**, 060401 (2016).
[3] M. R. Garey, D. S. Johnson, and L. Stockmeyer, Theor. Comput. Sci. **1**, 237 (1976).
[4] S. Popescu and D. Rohrlich, Found. Phys. **24**, 379 (1994).
[5] M. Navascués, S. Pironio, and A. Acín, New J. Phys. **10**, 073013 (2008).
[6] M. Navascués, A. Felix, M. Araujo, and T. Vertesi, Phys. Rev. A **92**, 042117 (2015).
[7] R. Colbeck and R. Renner, Nat. Phys. **8**, 450 (2012).
[8] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevA.97.020103 for detailed problem description, a proof sketch and the proofs of Theorems 1 and 2.
[9] S. Fiorini, S. Massar, S. Pokutta, H. R. Tiwary, and R. de Wolf, in *Proceedings of the 44th Symposium on Theory of Computing–STOC '12* (ACM, New York, 2012), pp. 95–106.
[10] J. Gouveia, P. A. Parrilo, and R. R. Thomas, Math. Oper. Res. **38**, 248 (2013).
[11] H. Fawzi, J. Gouveia, P. A. Parrilo, R. Z. Robinson, and R. R. Thomas, Math. Program. **153**, 133 (2015).
[12] Z. Ji, arXiv:1310.3794.
[13] S. Burgdorf, M. Laurent, and T. Piovesan, arXiv:1502.02842.
[14] C. Stark, Phys. Rev. A **89**, 052109 (2014).
[15] D. Rosset, R. Ferretti-Schöbitz, J.-D. Bancal, N. Gisin, and Y.-C. Liang, Phys. Rev. A **86**, 062325 (2012).
[16] C. J. Stark and A. W. Harrow, IEEE Trans. Inf. Theory **62**, 2867 (2016).
[17] R. Gallego, N. Brunner, C. Hadley, and A. Acín, Phys. Rev. Lett. **105**, 230501 (2010).
[18] N. Harrigan, T. Rudolph, and S. Aaronson, arXiv:0709.1149.
[19] S. Wehner, M. Christandl, and A. C. Doherty, Phys. Rev. A **78**, 062112 (2008).
[20] C. Stark, arXiv:1209.6499.
[21] C. Jackson and S. J. van Enk, Phys. Rev. A **92**, 042312 (2015).
[22] S. Kimmel and Y.-K. Liu, arXiv:1510.08887.
[23] S. T. Merkel, J. M. Gambetta, J. A. Smolin, S. Poletto, A. D. Córcoles, B. R. Johnson, C. A. Ryan, and M. Steffen, Phys. Rev. A **87**, 062119 (2013).
[24] R. Blume-Kohout, J. K. Gamble, E. Nielsen, J. Mizrahi, J. D. Sterk, and P. Maunz, arXiv:1310.4492.
[25] S. Kimmel, M. P. da Silva, C. A. Ryan, B. R. Johnson, and T. Ohki, Phys. Rev. X **4**, 011050 (2014).
[26] S. Kimmel, G. H. Low, and T. J. Yoder, Phys. Rev. A **92**, 062315 (2015).
[27] A. C. Dugas, J. Wallman, and J. Emerson, Phys. Rev. A **92**, 060302 (2015).
[28] A. Monras and A. Winter, J. Math. Phys. **57**, 015219 (2016).
[29] C. Stark, arXiv:1601.06035.
[30] T. S. Cubitt, J. Eisert, and M. M. Wolf, Phys. Rev. Lett. **108**, 120503 (2012).
[31] Á. Rivas, S. F. Huelga, and M. B. Plenio, Rep. Prog. Phys. **77**, 094001 (2014).
[32] J. P. Dehollain, J. T. Muhonen, R. Blume-Kohout, K. M. Rudinger, J. K. Gamble, E. Nielsen *et al.*, New J. Phys. **18**, 103018 (2016).
[33] P. Faist and R. Renner, Phys. Rev. Lett. **117**, 010404 (2016).
[34] R. Blume-Kohout, arXiv:1202.5270.
[35] M. Guţă, T. Kypraios, and I. Dryden, New J. Phys. **14**, 105002 (2012).
[36] S. J. Van Enk and R. Blume-Kohout, New J. Phys. **15**, 025024 (2013).
[37] C. Ferrie, New J. Phys. **16**, 093035 (2014).
[38] R. Peeters, Combinatorica **16**, 417 (1996).
[39] S. A. Vavasis, SIAM J. Optim. **20**, 1364 (2009).
[40] Y. Shitov, arXiv:1606.09065.
[41] T. Lee, Z. Wei, and R. de Wolf, arXiv:1407.4308.