Heralded Polynomial-Time Quantum State Tomography

Steven T. Flammia,1 David Gross,2 Stephen D. Bartlett,3 and Rolando Somma1

1Perimeter Institute for Theoretical Physics, Waterloo, Ontario, N2L 2Y5 Canada
2Institute for Theoretical Physics, Leibniz University Hannover, 30167 Hannover, Germany
3School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia
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We describe an algorithm for quantum state tomography that converges in polynomial time to an estimate, together with a rigorous error bound on the fidelity between the estimate and the true state. The result suggests that state tomography on large quantum systems may be much more feasible than the exponential size of state space suggests. In many situations, the correctness of the state estimate can be certified from the data alone, with no a priori assumptions on the form of the measured state.

Quantum state tomography (QST) — the process of estimating a quantum state using local measurements given a large number of copies — is an exceptionally daunting task. As it is typically formulated [1], simply to output an estimate for a generic state of \(n\) qubits would take exponential time in \(n\), given that there are an exponential number of coefficients in a generic state’s description. This is but one of several inefficiencies. Most quantum states have exponentially small amplitudes in almost every basis, so to distinguish any one of these amplitudes from zero takes exponential time. Assuming one were able to collect all of that data from an informationally complete measurement, one is left with the intractable computational task of inverting the measured frequencies to find an estimate of the state.

These barriers to performing efficient quantum tomography for generic states are not necessarily applicable to real-world situations, however, as the traditional representation of quantum states in terms of Hilbert space vectors and density matrices is in a sense too general. Indeed, states which occur in many practical situations are specified by a small number of parameters. An efficient description could be a polynomial-sized quantum circuit that outputs the state; or, in the case of thermodynamical equilibrium states, a bounded-interaction-range Hamiltonian and a temperature. This insight is not new: researchers in many-body physics and quantum information theory have found many classes of states which are described by a number of parameters scaling polynomially in \(n\) and which closely approximate the kind of states found in particular physical systems [2–8].

However, the question of whether these restricted classes can be put to use in a tomographic setting has remained largely open. Any result closing this gap should address three points: 1. Choose a few-parameter set of states adapted to the physical nature of the system under consideration. 2. Specify a protocol which efficiently [22] identifies these parameters from a small and simple-to-implement set of measurements. 3. If possible, give an independent way of verifying that the protocol produced a faithful estimate of the physical state (without having to assume that the set chosen in the first step correctly describes the system).

We briefly explain the third point. An experimentalist should be wary of any tomographic procedure for which the success is predicated on some abstract technical condition (e.g., the system is well-described by a “matrix product state of bond dimension \(D\)”). Therefore, it is desirable that the protocol infers from the data alone whether or not it can guarantee a faithful reconstruction, and aborts if it cannot. We say that such a procedure heralds its own success.

In this work, we address all three problems above by presenting an algorithm for heralded quantum state tomography using a polynomial amount (poly(\(n\))) of measurement and classical computation.

The physical system we have in mind is one where the constituents are arranged in a one-dimensional configuration (e.g. ions in a linear trap [9]). It is highly plausible that in such a setting, correlations between neighboring qubits are much more pronounced (due to direct interaction) than correlations between distant systems (mediated e.g. by global fluctuations of control fields). A polynomially-sized class of states anticipating exactly this behavior has long been studied under the names of finitely correlated states (FCS) or matrix product states (MPS) [2, 10]. Below, we present the heralded MPS tomography (H-MPS) algorithm. Given experimental data, it outputs either a polynomial-sized pure matrix product state together with a rigorous bound on the fidelity between the true density matrix and the estimate, or else it returns a failure flag. This happens in particular when such an efficient description does not exist. At least in an idealized scenario, one can guarantee that an efficient MPS description will be found in polynomial time, given that it exists.

In later sections, we sketch generalizations to higher dimensions, to highly mixed systems, and to quantum channels describing correlated noise. We emphasize that the H-MPS algorithm can be employed whenever one expects that an MPS description for a system may be appropriate, whether or not it possesses a one-dimensional geometry. Examples of MPS include the GHZ, W, cluster, and AKLT states. Our results also address an open...
question of Aaronson [11] by demonstrating that MPS

To find an unknown quantum state $\rho$ of $n$ qudits (d-

dimensional quantum systems), we propose the following

One selects a number $k \ll n$, such that obtaining an estimate for

We denote the reduction of $\rho$ to sites $j, j+1, \ldots, j+(2k-1)$ by $\rho_j$, and we use $\sigma_j$ to refer to a tomographic estimate

Assume that by standard methods one obtains a confidence interval such that, for all $j$, the trace norm of $\rho - \sigma_j$ is

with high confidence.

The data $\{\sigma_j, \epsilon_j\}$ are then passed to the H-MPS algorithm. It either declares a failure and aborts, or else outputs an efficiently describable state $|\Psi\rangle$ and a number $\tau$ such that the fidelity provably obeys

whenever (1) holds.

It may come as a surprise that such a certificate is possible. After all, there are exponentially many degrees of freedom which remain unmeasured in the procedure. How can we guarantee that there are no two orthogonal states which happen to coincide on the tiny number of coefficients we have obtained information about? Geometrically, the reason is that a generic MPS is “locally exposed” [2], i.e. it lies at an extreme point of the space of quantum states, whose tangent plane corresponds to a local functional. In physical terms: with every MPS, one can associate a gapped, local Hamiltonian, which acts as a witness for that state [2, 10]. The main technical issue solved below is finding a simple way of bounding this gap for finite, non-translationally invariant and possibly degenerate systems.

Before describing the algorithm, we pause to recall the definition of MPS [2, 10]. A state vector $|\Psi\rangle$ on $n$ qudits is an MPS with bond-dimension $D$ if there are $nd$ complex $D \times D$ matrices $\{A_j^s\}$, $s = 1, \ldots, d; j = 1, \ldots, n$ such that

$$|\Psi\rangle = \sum_{s_1, \ldots, s_n=1}^d \text{Tr}[A_1^{s_1}A_2^{s_2}\cdots A_n^{s_n}]|s_1, s_2, \ldots, s_n\rangle.$$ (3)

Here, $D$ is a free parameter which describes the complexity of the model. It is well-known that any state has an MPS description if one allows $D$ to scale exponentially with $n$. However, the motivation for the seemingly ad-hoc definition (3) stems from the fact that many natural states are well-approximate by an MPS with small $D$. Note there are only $nD^2$ parameters specifying $|\Psi\rangle$.

H-MPS. The algorithm consists of two steps. In the first stage, we compute an MPS estimate from the experimental data. The task of the second step is to certify the fidelity of the estimate. Because we will retrospectively verify the output of step one, it is not necessary to insist on theoretical guarantees on the performance of this part. Any ansatz, even an “educated guess”, can lead to a rigorous result, as long as it will be vindicated by passing the second stage of H-MPS. Therefore, we give a list of algorithms for finding MPS estimates below, without definitely endorsing one over the others. A more detailed study of practical performances will be provided elsewhere. For clarity of presentation, we will restrict attention to “generic” states at first, treating singular situations in the end.

The Variational Method. A natural way of obtaining FCS estimates from data is by way of a variational algorithm: note that the local reductions of an MPS can be computed efficiently. Therefore, it is feasible to change the matrices one at a time, so as to minimize the sum of the trace-norm differences between the measured estimates and the computed local reductions. Since the target function is bounded from below and reduced in every step, the algorithm will certainly converge. The advantage of this method is that all the available information is utilized, and that it is inherently stable against small noise. On the negative side, it may be prone to run into local minima. (We emphasize, however, that the algorithm should not be judged by the high standards of the variational methods employed in many-body physics, which reliably find the global minimum of energy functions on tens of thousands of spins. A density operator even on ten three-level “qutrits” depends on 3.4 billion coefficients. If the trace-norm distance can be reliably minimized for such comparatively tiny systems, it would make tomography possible in otherwise intractable regimes – even if the algorithms fails to scale to the orders of magnitude which are standard today in numerical condensed matter physics).

The Quantum 2-SAT Method. Recent developments in the context of the “quantum satisfiability problem” show that it is possible to directly and efficiently find the MPS description of the ground state space of a one-dimensional frustration-free Hamiltonian, provided that the following condition holds: for every $1 \leq j \leq n$, the degeneracy of the restriction of the Hamiltonian to sites $1$ to $j$ does not exceed a uniform bound. A qubit version described in [12] can be generalized to arbitrary situations [13]. It easily follows that – at least in the idealized scenario of vanishing experimental errors – reconstructing an MPS description given only information about the support of the reduced density operators (on a sufficiently large neighborhood) is provably efficient. While it is unclear whether this approach is well-suited for practical purposes, it shows that there are no computationally hard instances which would make any attempt of finding a general solution futile from the outset. This may be a surprising fact, given that hard instances are known to occur for more general frustration-free Hamiltonians with
compute the reduced density matrix of the estimate $\rho_j$. Let $\gamma_j$ be the square-root of the largest eigenvalue not equal to one. Set $\gamma = \max_j \gamma_j$. The H-MPS algorithm concludes by outputting $|\Psi\rangle$ and $\tau = \frac{1}{2^{D_j}} \sum_j (\text{Tr}(h_j \sigma_j) + \epsilon_j)$.

In the following paragraph we prove the validity of Eq. (2). The technical hurdle to overcome is to lower-bound the gap in the spectrum of $H = \sum_{j=1}^{n-1} h_j$. For non-degenerate translationally invariant (TI) systems, a (fairly involved) proof was given in [2]. Partly building on their ideas, we present a short argument below, which applies to the relevant case of finite, non-TI quantum states.

By construction, $H \geq 0, H \psi = 0$, so that the lowest eigenvalue of $H$ is zero. We claim that the second-smallest eigenvalue gap$(H)$ is lower-bounded by $(1 - 2\gamma)$. To prove the assertion, we start by following [2] and note that gap$(H) = \max \{ \lambda | H^2 \geq \lambda H \}$. Compute:

$$H^2 = \sum_{j=1}^{n-2} (h_j^2 + \sum_{j'=1}^{j-1} h_j h_{j+1}) + \sum_{\lvert j-j'\rvert \geq 1} h_j h_{j'} \geq H + \sum_{j=1}^{n-2} [h_j, h_{j+1}]_+, \tag{5}$$

where we used the fact that the $h_j$ are projections and omitted non-negative summands. Next, we will establish

$$[h_j, h_{j+1}]_+ = -\gamma_j (h_j + h_{j+1}). \tag{6}$$

We borrow some facts from basic Hilbert space theory [15, 16]: any two projection operators $h_j, h_{j+1}$ can be brought simultaneously into block diagonal form, where on the $i$th block, $h_j$ and $h_{j+1}$ act like one-dimensional projections whose ranges are vectors enclosing the canonical angle $\theta_i$. One verifies that $\cos^2 \theta_i$ is the $i$th eigenvalue of $h_j h_{j+1}$. Certainly (6) holds on the entire space if and only if that relation is true on every block. Thus, we have reduced the problem to the case of one-dimensional projectors in a two-dimensional space. Here, we can solve it by elementary means and find that (6) holds for non-trivial angles as long as $\gamma \geq \cos \theta_i$, which is true by construction. Plugging (6) into (5) gives

$$H^2 \geq H - \gamma \sum_j (h_j + h_{j+1}) \geq (1 - 2\gamma) H,$$

completing the proof of the gap estimate. To get the fidelity bound (2), label the eigenvectors of $H$ by $|E_i\rangle = |\Psi\rangle, |E_{i1}\rangle, \ldots |E_{in-1}\rangle$. We know that the eigenvalue $E_0$ equals zero. Since invertibility of the $\Gamma_j$’s guarantees uniqueness of the ground-state [2, 10], the bound on the gap ensures that all other eigenvalues fulfill $E_i \geq (1 - 2\gamma)$. Thus

$$\sum_j (\text{Tr}(h_j \sigma_j) + \epsilon_j) \geq \text{Tr}[H \rho]$$

$$= \sum_i E_i \langle E_i | \rho | E_i \rangle \geq (1 - 2\gamma)(1 - \langle \Psi | \rho | \Psi \rangle).$$
Finally, we remark that based on the ideas in \cite{2}, it can be shown that $\gamma \to 0$ exponentially fast as $k$ is increased.

\textit{Degeneracy and singular cases.} While the certification algorithm above works for “most” MPS states, it may fail in certain singular cases. The simplest example is given by the family of GHZ-type states $\frac{1}{\sqrt{2}} (|0, \ldots, 0\rangle + e^{i\phi} |1, \ldots, 1\rangle)$. Since any local reduced density matrix is independent of $\phi$, it is \textit{impossible} to distinguish the members of that family based on local information alone. (Indeed, for these states the $\Gamma_j$-operators defined above will not be invertible – so that an error would have been declared). However, one may verify that the simple “string operator” $\sigma_x \otimes \ldots \otimes \sigma_x$ has expectation value $\cos \phi$ for the states above. Thus, it is reasonable to expect that H-MPS can be extended, enabling it to learn (and certify) any MPS with bounded bond dimension.

It turns out that this possible, as we will briefly sketch now. Indeed, if the algorithm described above reports an error (i.e. if the $\Gamma_j$’s fail to be invertible), one would proceed as follows. Employing the Quantum 2-SAT Method, compute an MPS representation of the projector onto the ground space of the parent Hamiltonian of the estimate. It may happen that the dimension of this space grows exponentially as more sites are taken into account. In this case, H-MPS will have definitely failed (in the limit of vanishing noise, this only happens if no MPS description with given bond dimension exists). However, in many relevant situations, the dimension will saturate at a finite value. Re-examining the gap estimate above shows that (unlike the original proof in \cite{2}), it remains valid for models with a degenerate ground state space. Hence, at this point, we can certify the overlap between the true state and a small subspace of the exponentially large ambient space.

It remains to be shown that even this comparatively small ambiguity can be efficiently resolved. Treating all special cases which may appear in the most general situation is somewhat cumbersome and will be deferred to a future publication. Here, we restrict attention to the most relevant case: a two-fold degeneracy (this covers the GHZ and the W state). Formally, we are facing the task of performing tomography in a copy of $\mathbb{C}^2$, which has been embedded into $\mathbb{C}^d$. A classic result states that any two orthogonal pure states of a multi-partite system can be reliably distinguished using local operations alone \cite{17}. This holds true in particular for the embedded versions of the eigenvectors of the three Pauli matrices acting on $\mathbb{C}^2$. Therefore, the overlaps between a state in the ground-space and this informationally complete set of vectors may be found by local operations. We end the discussion by noting that the procedure equally applies to the case where $\rho$ is far from a pure state, as long as its support is contained in an MPS space.

\textit{Generalizations and Outlook.} The theory of MPS can be generalized to higher-dimensional configurations, where the resulting states are sometimes referred to as PEPS. We note that our gap estimate does not crucially rely on the geometry of the neighborhood relations. Therefore, conceptually, it should be relatively straightforward to generalize the basic techniques to these situations. However, efficiently finding good PEPS approximations to the data is likely to be extremely challenging.

While this Letter emphasized (approximately) pure states, tomography of highly mixed states may actually be more pertinent in realistic settings. If we drop the desire to certify the result, this task proves relatively simple. Recall that a mixed state $\rho$ is called \textit{finitely correlated} \cite{2} if the linear space of operators

$$\{\text{tr}_R[\rho A_R] \mid A_R \in \mathcal{B}(R)\}$$

has dimension smaller than some fixed constant $D^2$, where the indices $L, R$ refer to a bi-section of the chain into a left and a right part. The symbol $\mathcal{B}(R)$ denotes the set of all operators acting on the right hand side (r.h.s). Physically, the definition says that there are only $D^2$ ways of modifying the state on the l.h.s. by conditioning on an event taking place on the r.h.s. of the chain. It has been shown in \cite{2} that any state with that property has an efficient representation, and once again it is natural to ask whether this small set of parameters can be experimentally obtained, and whether success can be certified without technical assumptions. Under a mild invertibility assumption akin to (4), the answer to the first question turns out to be affirmative. While details will be provided elsewhere, we briefly list the main features of
the algorithm: It is guaranteed to obtain a faithful representation, without the need for any optimizations or variational calculations; it yields a representation which may be used to predict the expectation value of any (of the exponentially many) factorizing observables, even though only (linearly many) local observables were measured to find the estimate. The MPS pure states discussed above are included as a special case. On the downside, the resulting “matrix product operators” are much harder to interpret; there is no way of heralding errors if the assumptions are not met and the resulting state will be non-negative only within the margins of experimental accuracy.

We remark that our the results on mixed state tomography immediately generalize to quantum process tomography. The analogue of a non-factoring quantum state is here a channel with correlations over many uses, while the analogue of the FCS representation are channels with memory [18]. Obtaining the parameters of these objects efficiently is, courtesy of the Choi-Jamiolkowski isomorphism, just as straight-forward as learning mixed FCS.

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Note added. After the research for this work had been completed [19], the authors learned that two independent groups had worked along similar lines.

Let us compare the present work with the recent work in Ref. [20]. Conceptually, the two contributions seem very close. Both make the point that tomography of many-body quantum systems may not be as impossible as it superficially seems. But the respective technical focus is quite different. While Ref. [20] puts forward a new algorithm for finding MPS approximations given measured data, we emphasize methods for certifying that the estimate is actually correct. Employing the MPS-SVT method of Ref. [20] in step one of our H-MPS algorithm, it should be possible to seamlessly combine the two results.

Unrelatedly, the authors were recently made aware of the fact that a further group was preparing results [21] on the problem presented here.