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Quantum System Identification

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The aim of quantum system identification is to estimate the ingredients inside a black box, in which some quantum-mechanical unitary process takes place, by just looking at its input-output behavior. Here we establish a basic and general framework for quantum system identification, that allows us to classify how much knowledge about the quantum system is attainable, in principle, from a given experimental setup. We show that controllable closed quantum systems can be estimated up to unitary conjugation. Prior knowledge on some elements of the black box helps the system identification. We present an example in which a Bell measurement is more efficient to identify the system. When the topology of the system is known, the framework enables us to establish a general criterion for the estimability of the coupling constants in its Hamiltonian.

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Some of the most exciting and puzzling concepts in quantum theory can already be observed in simple systems. These are, for example, superpositions and decoherence, tunneling, entanglement and nonlocality, quantum cryptography, teleportation, and dense coding. Many such theoretical ideas have been confirmed experimentally with tremendous accuracy. On the other hand, perhaps the most important theoretical concept—a full quantum computer or simulator—is still well out of reach, because it requires a fully controllable system of Hilbert space dimension at the very least of the order of \(2^{100}\). Its realization poses one of the greatest challenges in science.

On our path towards quantum computation we are building systems composed of more and more qubits, the quantum information theoretic equivalent of the bit. But while an information theoretic approach is very successful, we should not forget that any implementation comes with a baggage of physical effects. In particular, real qubits interact. Often, these interactions are important: they are actively used to create logical gates. Sometimes, they are unwanted, and either suppressed actively, or simply neglected. However, if we are to meet the stringent bounds that fault-tolerance computation puts on the required precision of our technology, we will have to estimate our quantum system with very high precision. Current estimates of the fault-tolerance threshold indicate that in many systems the relative precision will have to be of the order of \(10^{-3}–10^{-4}\).

If we could perfectly control our system, achieving such precisions is a mere engineering difficulty. But if our control relies on the system couplings, or is heavily perturbed by them, we are in a catch-22 situation, and it is unclear how well the system can be estimated even in principle. In this Letter, we solve this question by providing a precise mathematical description of the equivalent set \([1–3]\) of closed systems. This set describes the possible implementations of a system that cannot be distinguished with a given experimental setup. It should be compared to the well-known reachable set in quantum control \([4]\), which describes the set of unitary operations that can be implemented, in principle, by a given experimental setup.

It has been shown in quantum control that even when only parts of the system are accessed, the reachable set typically remains maximal: the system is capable of quantum computation \([5]\). We show that this is not true for full estimability: in general, infinitely many different system Hamiltonians give rise to the same input-output behavior. However, we show how \(a\) pri\(or\) knowledge about the system helps to restrict the set of possible systems. Indeed we prove that in a generic limited-access situation, relatively little \(a\) pri\(or\) knowledge can imply full estimability. This generalizes several recently developed schemes for indirect estimation \([6–9]\). We also show how estimability can strongly depend on the structure of quantum measurements, by providing an example where entangled observables are more efficient for the estimation than product observables.

Our analysis first follows closely the known results from bilinear theory \([1]\). Then, we use a result from Lie algebras \([10]\) to translate the bilinear theory to the quantum case. This sets our result apart from previous work which required additional mathematical assumptions \([2,3]\).

Setup.—We consider a black box with \(N_i\) inputs and \(N_o\) outputs. Inside the black box, some quantum-mechanical unitary dynamics takes place. Our goal is to find a model for the black box that perfectly describes its input-output behavior under all possible circumstances (system identification \([1]\)).

More specifically, we are modeling a system with a finite-dimensional Hilbert space \(\mathcal{H}\), a time dependent Hamiltonian
\[ H(t) = H_0 + \sum_{k=1}^{N_i} f_k(t) H_k, \]

an initial quantum state \( \rho_0 \), and a set of observables \( M_\ell \) (\( \ell = 1, \ldots, N_o \)). Without loss of generality we chose \( H_0 \) and \( H_k \) traceless. The inputs are the functions \( f_k(t) \) (\( k = 1, \ldots, N_i \)), which are assumed to be piecewise constant. The outputs are the expectation values of the observables \( M_\ell \),

\[ \text{tr} \{ M_\ell \rho(t) \} \quad \text{with} \quad \rho(t) = T - \exp \left( \int_0^t dt' \mathcal{L}(t') \right) \rho_0, \]

where

\[ \mathcal{L}(t) = \mathcal{L}_0 + \sum_{k=1}^{N_i} f_k(t) \mathcal{L}_k, \]

\[ \mathcal{L}_k = -i[H_k, \cdot] \quad (k = 0, \ldots, N_i) \]

are the Liouvillians corresponding to the Hamiltonians. See Fig. 1. Because we are interested in whether systems can be distinguished in principle, we assume that it is possible to collect statistics at arbitrary precision, and that infinitely many copies of the system are available (this allows us to ignore any backaction of the measurements \([2,3]\)). Our main assumption is that the system is controllable, implying that any unitary transformation can be realized by the Hamiltonian dynamics with \( H(t) \), by properly arranging the inputs \( f_k(t) \). Mathematically this amounts to the smallest Lie algebra over the reals that contains the matrices \( iH_0, iH_1, \ldots, iH_{N_i} \) being equal to the full Lie algebra \( \text{su}(\text{dim} \mathcal{H}) \) of traceless skew-Hermitian matrices of size \( \text{dim} \mathcal{H} \times \text{dim} \mathcal{H} \). Controllability is a generic property of systems, as two randomly chosen Hermitian operators are almost surely universal for quantum computing \([5]\), even when only physical Hamiltonians are picked \([11]\). In addition, the controllability is in principle an observable property, if the dimension of the underlying Hilbert space is known. Furthermore, we exclude the trivial cases where \( M_\ell \) or \( \rho_0 \) is proportional to the identity operator.

We put all parameters together in the system \( \sigma = \{ H_0, H_k, M_\ell, \rho_0 \} \). Two systems \( \sigma \) and \( \tilde{\sigma} \) are called equivalent \([1]\), if they are indistinguishable by all input-output experiments. Therefore by definition, we can estimate the real system \( \sigma \) up to equivalence. Let us call the estimated system \( \tilde{\sigma} \), which consists of estimated components \( \tilde{\sigma} = \{ \tilde{H}_0, \tilde{H}_k, \tilde{M}_\ell, \tilde{\rho}_0 \} \). We assume that the estimated system has been chosen to be of minimal dimension, which implies that this system is also controllable. The goal now is to find a mathematical description of how different \( \tilde{\sigma} \) can be from the real system \( \sigma \).

**Equivalence and similarity.**—First, we have to find a mathematical description of the equivalence. For some fixed input, equivalence means that the real system and the estimated system have to agree on all observable outputs for all times, i.e.,

\[ \text{tr} \{ M_\ell \rho(t) \} = \text{tr} \{ \tilde{M}_\ell \tilde{\rho}(t) \}, \]

where \( \tilde{\rho}(t) \) is the state evolving from the initial state \( \tilde{\rho}_0 \) with the Hamiltonians \( \tilde{H}_0 \) and \( \tilde{H}_k \). This is not very useful mathematically, because it still involves solving the Schrödinger equation. There is an algebraic description of this property that is much easier. Let us denote \( \mathcal{L}_\alpha = \mathcal{L}_{\alpha_1} \cdots \mathcal{L}_{\alpha_n} \) with the Hamiltonians \( \tilde{H}_0 \) and \( \tilde{H}_k \), where \( \alpha \) is a multi-index of length \( L \) with entries \( \alpha_j \in \{0, \ldots, N_i\} \). Further, we include the case \( L = 0 \) as the identity superoperator and introduce similar notation \( \tilde{\mathcal{L}}_\alpha \) for the estimated system. Equivalence can then be formulated as

\[ \text{tr} \{ M_\ell \mathcal{L}_\alpha \rho_0 \} = \text{tr} \{ \tilde{M}_\ell \tilde{\mathcal{L}}_\alpha \tilde{\rho}_0 \}, \]

for any multi-index \( \alpha \). This can be thought of as an “infinitesimal version” of (1), and a simple proof of this statement is found in \([2]\).

We call systems similar if and only if there is a similarity transformation between them

\[ \mathcal{L}_k = \mathcal{T} \tilde{\mathcal{L}}_k \mathcal{T}^{-1}, \quad \mathcal{M}_\ell = \tilde{\mathcal{M}}_\ell \mathcal{T}^{-1}, \quad \rho_0 = \mathcal{T} \tilde{\rho}_0 \]

(3)

\( (k = 0, \ldots, N_i) \), where \( \mathcal{M}_\ell \) and \( \tilde{\mathcal{M}}_\ell \) represent the actions of \( M_\ell \) and \( \tilde{M}_\ell \) in the Liouville space. It is obvious that similarity implies equivalence. Similarity is much easier to handle than equivalence, because of its simple mathematical structure.

**Translation to quantum case.**—In bilinear system theory \([1]\), it was shown that if \( \sigma \) is controllable then equivalence implies similarity. This is proven by explicit construction of the similarity transformation between \( \sigma \) and \( \tilde{\sigma} \). Because there are some subtle differences in the quantum case, we briefly repeat these arguments.

Assume \( \sigma \) and \( \tilde{\sigma} \) are equivalent and pick an arbitrary state \( \tilde{\rho} \). We show that due to the controllability of system \( \tilde{\sigma} \), the state \( \tilde{\rho} \) can be expressed as

\[ \tilde{\rho} = \sum_\alpha \lambda_\alpha \tilde{\mathcal{L}}_\alpha \tilde{\rho}_0. \]

First, because \( i\tilde{\rho}_0 \in \mathfrak{u}(\text{dim} \mathcal{H}) \) (the algebra of skew-Hermitian matrices) the set \( R = \{ iA | A = \sum_\alpha \lambda_\alpha \tilde{\mathcal{L}}_\alpha \tilde{\rho}_0 \} \) is...
a subset of \(u(\text{dim} \mathcal{H})\). Because \(i[\hat{L}_k, \hat{L}_j]\) and we have controllability, the linear combinations of \(\hat{L}_a\) include \(L_{\hat{H}} = -i[\hat{H}, \cdot]\) for any Hermitian \(\hat{H}\). This means that \([i\hat{H}, iA] \in R\), so \(R\) is an ideal. Because it is not equal to the identity and not \(su(\text{dim} \mathcal{H})\), we must have \(R = u(\text{dim} \mathcal{H})\). Therefore, we can express any Hermitian operator as \(\sum a_{\alpha} L_a \hat{\rho}_0\), and, in particular, any state \(\hat{\rho}\), as in (4).

We then define \(\mathcal{T}\) by

\[
\mathcal{T} \hat{\rho} = \sum a_{\alpha} L_a \hat{\rho}_0.
\]

There are many possible representations of \(\hat{\rho}\). In order to see that \(\mathcal{T}\) is well-defined as a mapping, we need to verify that any two equal representations \(\sum a_{\alpha} L_a \hat{\rho}_0 = \sum a_{\beta} L_\beta \hat{\rho}_0\) imply \(\sum a_{\alpha} L_a \hat{\rho}_0 = \sum a_{\alpha} L_a \hat{\rho}_0\). By linearity, it is enough to show that

\[
\sum a_{\alpha} \hat{L}_a \hat{\rho}_0 = 0 \Rightarrow \sum a_{\alpha} L_a \hat{\rho}_0 = 0. \quad (5)
\]

Suppose that \(\sum a_{\alpha} L_a \hat{\rho}_0 = 0\). Then, we have for any \(\beta\)

\[
\text{tr}\left[\hat{M}_\beta \sum a_{\alpha} \hat{L}_a \hat{\rho}_0\right] = \sum a_{\alpha} \text{tr}[\hat{M}_\beta L_\beta \hat{\rho}_0] = 0,
\]

where \(\hat{L}_a \hat{\rho}_0 = \hat{L}_a \hat{\rho}_0\). Now, due to the input-output equivalence (2) between the two systems \(\alpha\) and \(\beta\), i.e.,

\[
\text{tr}[\hat{M}_\beta \hat{L}_a \hat{\rho}_0] = \text{tr}[M_\beta L_\beta \hat{\rho}_0] \quad \text{for any } \beta \alpha,
\]

we get

\[
\text{tr}\left[\hat{M}_\beta \sum a_{\alpha} L_a \hat{\rho}_0\right] = \sum a_{\alpha} \text{tr}[M_\beta L_\beta \hat{\rho}_0] = 0.
\]

Since this holds for any \(\beta\) and the system is controllable, we conclude \(\sum a_{\alpha} L_a \hat{\rho}_0 = 0\), which completes the proof of (5). The mapping is onto due to the controllability of the system, and is shown to be one-to-one by reversing the argument which proved that it is well defined. Finally, using controllability and the property \(\mathcal{T} \hat{\rho}_0 = \rho_0\), it is easy to see that \(\mathcal{T}\) has to fulfill (3).

**Unitarity.**—Since we restrict ourselves to unitary dynamics, it is possible to prove that the above similarity \(S(\cdot) \equiv \mathcal{T} \cdot \mathcal{T}^{-1}\) is actually inducing a unitary transformation on Hamiltonians. First, we note that both the real and the estimated Liouvillians have the commutator structure \(L_k = -i[H_k, \cdot]\) and \(\hat{L}_k = -i[\hat{H}_k, \cdot]\), since we restrict ourselves to unitary dynamics. These Liouvillians form a subspace \(\mathcal{U}\) of all possible Liouvillians. We first show that controllability implies that this subspace is mapped into itself by the similarity transformation \(S\). Indeed, a simple expansion of commutators combined with \(S\) being a similarity transformation shows that

\[
S(-i[\hat{H}_k, \hat{H}_j], \cdot) = S(i[\hat{L}_k, \hat{L}_j]) = i[\hat{L}_k, \hat{L}_j] = -i[[H_k, H_j], \cdot] \in \mathcal{U}.
\]

By linearity, any element \(\hat{H}\) of the generated algebra has the property that \(S(-i[\hat{H}, \cdot]) \in \mathcal{U}\). Because the system is controllable, this algebra is just the set of all traceless Hermitian matrices, and therefore \(S(\mathcal{U}) = \mathcal{U}\). Since there is an isomorphism between \(L_{\hat{H}} = -i[\hat{H}, \cdot]\) and \(\hat{H}\), we can represent the action of \(S\) on \(\mathcal{U}\) by a corresponding action on \(su(\text{dim} \mathcal{H})\). By linearity, this must be a linear and invertible map \(S\). Indeed, from (6) it follows that \(S([\hat{H}, \hat{H}^\dagger]) = [S(\hat{H}), S(\hat{H}^\dagger)]\); \(S\) is a Lie automorphism. A theorem in [10] states that all automorphisms on \(gl(n)\) (the general matrix algebra) are of the form \(S(X) = AXA^{-1}\) or \(S(X) = -AX^T A^{-1}\). Our automorphism is instead on the subalgebra \(su(\text{dim} \mathcal{H})\). By choosing a Hermitian basis of \(gl(n)\) we can extend it uniquely to one of \(gl(n)\) and apply the theorem. The additional Hermitian structure demands, furthermore, that \(A^{-1} = A^\dagger\). Thus, \(S(\hat{H}) = U \hat{H} U^\dagger\) or \(S(\hat{H}) = -U \hat{H}^T U^\dagger\). The latter is excluded because it would not preserve the trace of quantum states. Hence, under the premise of controllability, two systems are indistinguishable if and only if they are related through a unitary transformation

\[
H_k = U \hat{H}_k U^\dagger, \quad M_\ell = U \hat{M}_\ell U^\dagger, \quad \rho_0 = U \hat{\rho}_0 U^\dagger.
\]

**Usage of a priori knowledge.**—In practice, it is reasonable to assume that some elements of the black box are known. Each known element shrinks the set of possible unitary transformations, because, for example, \(H_k = U \hat{H}_k U^\dagger\) implies \(U \hat{H}_k U^\dagger = \hat{H}_k\) implies \([U, \hat{H}_k] = 0\).

As an example, we consider two qubits coupled by an unknown Hamiltonian. We estimate them by performing arbitrary operations \(\hat{H}_1 = X_1 \otimes 1_2\) and \(\hat{H}_2 = Y_1 \otimes 1_2\) on the first qubit and by measuring (a) \(Z_1 \otimes 1_2\), (b) \(1_1 \otimes Z_2\), or (c) \(|\Psi^\dagger\rangle_{12} \langle\Psi^-|\), where \(X_1, Y_1,\) and \(Z_1\) are the Pauli operators of qubit \(i = 1, 2\), and \(|\Psi^\dagger\rangle_{12} = (|01\rangle_{12} - |10\rangle_{12})/\sqrt{2}\) is the singlet state. Assuming that the system is controllable, we can apply the above results.

First, the conditions \([U, \hat{H}_1] = 0\) reduce the unitary transformation \(U\) to \(1_1 \otimes 1_2\). If \(U_2\) is a unitary operator acting on the second qubit, which may be parametrized as \(U_2 = e^{-i/2\alpha n \cdot \sigma_2}\) with a unit vector \(n\). We then impose another condition \([U, \hat{M}] = 0\):

(a) In the first case with \(\hat{M} = Z_1 \otimes 1_2\), this condition is already satisfied and the unitary transformation \(U\) is not reduced any further, \(U = 1_1 \otimes e^{-i/2\alpha n \cdot \sigma_2}\), where remain three parameters.

(b) In the second case with \(\hat{M} = Z_1 \otimes Z_2\), the condition reduces \(U\) to \(1_1 \otimes e^{-i/2\alpha n \cdot \sigma_2}\) with a single parameter.

(c) Finally, in the third case with \(\hat{M} = |\Psi^\dagger\rangle \langle\Psi^-|\), we have

\[
[U, \hat{M}] = i \sin \frac{\theta}{2} (n_y |\Psi^\dagger\rangle \langle\Psi^-| - n_x |\Phi^-\rangle \langle\Phi^-|) + \text{H.c.}
\]
which is vanishing only when \( \sin(\theta/2) = 0 \), i.e., \( U = I \) up to an irrelevant phase. This shows that the Bell measurement is more efficient to estimate the system.

**Infection criterion for arbitrary systems.**—Let us consider another more general example, a generic Hamiltonian of a \( d \)-dimensional Hilbert space in the form

\[
H_0 = \sum_{(n,m) \in E} c_{nm} |n\rangle \langle m|,
\]

where the orthonormal basis \( |n\rangle \) may be thought of as “local,” and \( E \) are the edges of the graph \( G = (|n\rangle, E) \), that describes the nonzero off-diagonal \( (n \neq m) \) couplings \( c_{nm} \). We assume that a set of nodes \( C \) can be controlled \( (H_0 = |k\rangle \langle k|, k \in C) \), and that some observable can be measured. The crucial assumption about the set \( C \) is that it is “infecting” \( G \) [7]. This property is defined by the following propagation rules: (1) \( C \) is “infected”; (2) infected nodes remain infected; and (3) the infection propagates from an infected node to a “healthy” neighbor if it is its only healthy neighbor. For an arbitrary Hamiltonian we can always find an infecting set; how many nodes it contains depends on how sparse the Hamiltonian is in the particular basis of consideration. In practice there are physical choices of the basis corresponding to local operations, and many Hamiltonians are infected by acting on a vanishing fraction of nodes only.

Based on the assumption that \( C \) is infecting, one finds that the system is controllable, so our theorem can be applied. First, there is a \( k \in C \) that has a unique neighbor \( \ell \) outside \( C \). For that \( k \) we have \( \{iH_k, iH_0\} = -\sum_{m \in n(k)} (c_{km}|k\rangle \langle m| - c_{mk}|m\rangle \langle k|) \), where \( n(k) \) is the neighborhood of \( k \). Commuting it with \( iH_k \) again yields

\[
\{[iH_k, iH_0], iH_k\} = i \sum_{m \in n(k)} (c_{km}|k\rangle \langle m| + c_{mk}|m\rangle \langle k|).
\]

For \( m \in n(k) \cap C \), on the other hand, we can single out terms by

\[
\{[iH_m, iH_0], iH_k\} = -i(c_{km}|k\rangle \langle m| + c_{mk}|m\rangle \langle k|).
\]

By adding these to (8) for all \( m \in n(k) \cap C \), only a single term \( i(\epsilon (c_{\ell k}|k\rangle \langle \ell| + c_{\ell k}|\ell\rangle \langle k|) \) is left. Commuting this with \( iH_k \) again gives \( c_{\ell k}|k\rangle \langle \ell| - c_{\ell k}|\ell\rangle \langle k| \). Finally, commuting the latter two and subtracting the term proportional to \( iH_k \) we are left with \( i(\epsilon |\ell\rangle \langle \ell| \) By induction, we can obtain \( |n\rangle \langle n| \) for any \( n \). This implies full controllability [12].

If we assume that the \( H_k \) are known, we need to look at the unitaries that commute with these operators. There will be many. However, we will assume here the knowledge that the Hamiltonian \( H_0 \) has the form given in (7). Hence, we are talking about an indirect coupling strength estimation [6–9], where the topology \( E \) is known while the parameters are unknown. Let us see what this knowledge implies. First, we have to have \( \{H_k, U\} = 0 = -[H_k, U^\dagger] \) \( (k \in C) \). Since \( H_k \) are projectors, that implies that \( |k\rangle \) must be an eigenstate of \( U \) and \( U^\dagger \) for all \( k \in C \). The estimated Hamiltonian \( \hat{H}_0 = U H_0 U^\dagger \) has to be of the form \( \hat{H}_0 = \sum_{(n,m) \in E} \hat{c}_{nm} |n\rangle \langle m| \), where \( \hat{c}_{nm} \) are unequal to zero and could in principle differ from \( c_{nm} \). The edges \( E \) must be the same for both \( H_0 \) and \( \hat{H}_0 \) because we assume knowledge of the topology. Because \( C \) is an infecting set, there is one \( k \in C \) that has a unique neighbor \( \ell \) outside of \( C \). The corresponding term in the Hamiltonian \( H_0 \) is

\[
c_{\ell k}|k\rangle \langle \ell| + \hat{c}_{\ell k}|\ell\rangle \langle k| \)
\]

for \( \ell \) that describes the nonzero off-diagonal \( (n \neq m) \) couplings \( c_{nm} \). This implies full controllability [12]. Finally, by induction we get that \( U \) must be a diagonal matrix in the “local” basis \( |n\rangle \). Thus, up to the local phases of the basis vectors the Hamiltonian \( H_0 \) is uniquely estimated. What is remarkable here is that we do not have to assume knowledge of the observable and the phases of \( c_{nm} \). This generalizes the previous results [6–9] substantially.

**Final remarks and future perspectives.**—An immediate question is how our result would generalize to open-system dynamics, e.g., in case environmental degrees of freedom are hidden and the system dynamics in the black box is perturbed by the noise. Even in such a case, we would be able to find a set of models of open-system dynamics that explain the input-output behavior of the black box consistently. But, in order to clarify how ambiguous the estimated systems are, we need controllability in the open system. An algebraic description of controllability in open systems is, however, a long-standing unsolved problem [13]. In any case, it is important to investigate how much we can do in the presence of noise.

A more promising outlook is to connect our results with quantum estimation theory [14] for finitely many samples. The accuracy of the system identification is affected by the standard error arising from the finiteness of the number of samples. In light of this, it would be interesting to explore how quantum metrology (the enhancement of the efficiency in the estimation with the help of entanglement) [15] is extended to the system identification, and it deserves consideration.

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