Quantum certification and benchmarking

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Concomitant with the rapid development of quantum technologies, challenging demands arise concerning the certification and characterization of devices. The promises of the field can only be achieved if stringent levels of precision of components can be reached and their functioning guaranteed. This Expert Recommendation provides a brief overview of the known characterization methods of certification, benchmarking, and tomographic recovery of quantum states and processes, as well as their applications in quantum computing, simulation, and communication.

a. Introduction. Recent years have seen a rapid development of quantum technologies, promising new real-world applications in communication, simulation, sensing and computation [4]. Quantum internet infrastructure enables unconditionally secure transmission and manipulation of information. Highly engineered quantum devices allow for the simulation of complex quantum matter. While noisy intermediate scale quantum devices will soon demonstrate a quantum advantage beyond the reach of any classical simulation, a longer term perspective of fault tolerant quantum computers aims to solve impactful problems from industry that are out of reach for classical computers. These prospects come along with enormously challenging prescriptions concerning the precision with which the components of the quantum devices function. The task of ensuring the correct functioning of a quantum device and the validation of the accuracy of the output, is referred to as certification or sometimes verification.

The very tasks of certification and benchmarking are challenged by intrinsic quantum features: The involved configurations spaces have enormous dimensions, a serious burden for any characterization. What is more, certification comes along with an ironic twist: It is highly non-trivial in light of the fact that certain quantum computations are expected to exponentially outperform any attempt at classically solving the same problem. While a large-scale universal quantum computers are still out of reach, already today do we have access to quantum simulators, that is, special-purpose, highly controlled quantum devices aimed at simulating physical systems. And, indeed, for such systems, often, no efficient classical simulation algorithm is available. As a consequence, as quantum devices are scaled up to large system sizes, application-specific tools of certification are required that go beyond standard approaches such as re-simulating a device on a classical computer or full tomographic reconstruction. It is such specifically ‘quantum’ certification tools that this Expert Recommendation summarizes and puts into context.

To do so, we offer a framework in which the resource cost as well as the assumptions made in such approaches are cast very naturally. We recommend that the resource cost and assumptions made in such approaches be specified explicitly in future method development. We then sketch different approaches to quantum certification, ranging from advanced tomographic tools such as compressed sensing, to fidelity estimation and witnessing and the verification of arbitrary quantum computations in an interactive fashion. The methods we sketch are crucial both for the development of noisy intermediate-scale quantum devices and quantum simulators that are available now or will become so in the near term, as well as for more sophisticated computing devices that might become available in the long term. We note that given existing reviews on various aspects of fully malicious verification schemes for powerful untrusted servers [35, 40], here we focus more on complementary aspects of certification in less adversarial settings from the perspective of quantum technologies.

b. Classifying quantum certification. In any task of quantum certification, the core aim is to establish the correct
functioning of a quantum device. Given the enormous effort of a full tomographic characterization of quantum states and processes, in many practical applications, protocols for certification will necessarily be constrained in the available resources and at the same time governed by the advice one hopes to gain from the protocol. With this in mind, it is instructive to conceptualize the quantum certification problem as a protocol between the quantum device, seen as being powerful, and its user, who is restricted in her or his measurement devices and computational power. One can classify schemes according to the effort and information gained, as well as in the assumptions made on the device and its user (see Fig. 1). Ultimately, even when one aims for tomographic knowledge, one may conceive of certification as a protocol that outputs ‘accept’ if the device functions correctly, and ‘reject’ if it does not. Whether the protocol accepts or rejects is determined according to reasonable measures of quality that are appropriate for the respective property of the device being certified (BOX 1).

The assumptions made on the devices and their users depend, among other aspects, on one’s trust levels and the specific setting at hand. Typically, which assumptions are made also has an effect on the protocol’s complexity in one way or the other, or even renders certification feasible in the first place. Conceptually speaking, there are three building blocks entering, each of which equipped with certain assumptions. This is, firstly, the quantum device to be certified, a distinct and often physically separate entity. In experimental scenarios it is commonly reasonable to include knowledge concerning the underlying physical mechanism and potential sources of error in terms of an adequate modelling framework. However, it can also make sense to merely assume that the device is a quantum mechanical object. Secondly, it is useful to distinguish the quantum measurement apparatus used in the characterization, which might include state preparation and short circuits. In an idealized setting, they may be assumed to be perfect. More practically relevant are situations in which one has a solid understanding of their functioning and characterized their efficiencies to some level. In many physical architectures, in particular in key platforms for quantum simulation, one can perform certain quantum measurements very accurately, but is severely limited in the type of measurements that can be performed. Thirdly, and finally, there is the classical data processing which consumes storage capacity and processing time. Ultimately, any characterization provides classical numbers. The device-independent setting makes no assumptions at all about the measurement apparatus and the device, taking into account the final data only. Such a setting is adequate, for example, if the device is a remote and untrusted quantum device that may be accessible only through the cloud.

The effort or complexity of such a certification protocol can be divided into several distinct parts: This is the number of different settings or rounds in which data is obtained from the device (measurement complexity). Implementing those different settings might require different quantum computational effort as for example quantified by the length of the circuit that implements a certain measurement. Then, there is a minimal number of experiments and resulting samples that need to be obtained for a protocol to meaningfully succeed (sample complexity). Finally, one needs to process those samples involving classical computational effort in time and space (postprocessing complexity).

Often, the complexity of a protocol can be traded for the amount of information about the device that the user can extract when running the protocol. Such information is crucial when it comes to designing and improving a concrete experimental setup, while it may be less important when the user’s goal is merely to check the correct functioning of, say, a newly bought device, or a remote server.

We now present and assess various tools for characterization ordered according to, first, the information that may be extracted from the protocol, and, second, the assumptions made in the protocol. In addition to the main text, we provide a tabular overview in which we quantitatively assess exemplary certification protocols for applications in cloud computing, demonstrating a quantum advantage, and quantum simulation and computation according to our classification (TA-
c. Certification protocols. In many scenarios, it is reasonable to assume that one’s quantum measurements are rather well characterized and that the object of interest is either a quantum state or process that can be accessed in independently identically distributed (i.i.d.) experiments. These assumptions are often very natural in laboratory settings in which the quantum device can be directly accessed. They are therefore at the heart of many characterization protocols and shall be our starting point for now.

The most powerful but at the same time most resource-intense such technique of certification is full quantum tomography [51, 54]. Here, the idea is to obtain knowledge of the full quantum state or process by performing sufficiently many (trusted) measurements. Given tomographic data, one can in particular obtain a certificate that the state lies in some region in state space. For many years such regions were typically constructed heuristically by first applying maximum likelihood estimation to construct a point estimate of the state [52] and then using resampling techniques to obtain error bars. More recently, techniques to obtain more rigorous region estimates have appeared including Bayesian credibility regions [11, 33] and confidence regions [12, 23, 99] where the former are usually smaller but depend strongly upon the Bayesian prior. Most importantly, from these tomographic reconstructions, one exactly learns the nature of deviation of the imperfect implementation to the target. Such data proves crucial when designing experimental setups as it yields information about the particular sources of errors present in the setup and hence functions as ‘actionable advice’ on how to improve the setup.

However, generic quantum state and process tomography is excessively costly in the size of the quantum system. Fortunately, many quantum states and processes that are encountered in realistic experiments exhibit significant structure: States are often close to being pure or have approximately low rank, so that methods of compressed sensing tomography [43, 46, 56] can be applied in which less resource expensive or more reliable recovery is possible based on the same type of (but randomly chosen) measurements compared to full tomography. Similarly, quantum processes are often close to being unitary [37, 58]. For local Hamiltonian systems, even further structure of locality comes into play. In particular, tensor network states can provide meaningful variational sets for tensor network tomography, which basically makes the structural assumption that there is little entanglement in the state, an assumption that is often valid for quantum many-body states to an extraordinarily good approximation [8, 25, 53, 73]. Also, variational sets inspired by machine learning have been considered [92]. In such situations, the effort of quantum state and process tomography can be significantly reduced. At least for intermediate-sized systems, such techniques are practically highly important.

If one is only interested in certain properties of a quantum state or process one may resort to so-called learning techniques, which scale much more favourably. For instance, one may merely be interested in probably approximately correctly (PAC) learning the expected outcomes of a certain set of measurements, e.g., local observables on the quantum state. PAC learning is possible with a measurement complexity that scales only linearly (in the number of qubits) in certain settings [1, 81, 82] but still incurs exponential computational effort. In another instance of learning, one might be confident that the given data is described by a certain restricted Hamiltonian (or Liouvillian) model whose parameters are however not known. Hamiltonian (or Liouvillian) learning techniques solve this task and recover the Hamiltonian parameters from certain data [42, 50].

In contrast to the abovementioned tools for characterizing a quantum device, fidelity estimation aims merely at determining the overlap of the actual quantum state or process implemented in a given setup with the ideal one. While fidelity estimation yields much less information than full tomography, one saves tremendously in measurement and sample complexity. In fact, using importance sampling one can estimate the fidelity of an imperfect preparation of certain pure quantum states in constant measurement complexity [38].

A yet weaker notion than fidelity estimation is fidelity witnessing. The idea of a fidelity witness is to cut a hyperplane through quantum state space which separates states close in fidelity to a target state from those far away. Efficient fidelity witnesses can often be derived in settings in which the target state satisfies some extremality property so that it lies in a low-dimensional corner of state space, such as certain multipartite entangled states [75], Gaussian bosonic states [5] or ground states of local Hamiltonians [48].

A still weaker approach merely aims at verifying or estimating the presence of certain key properties, such as entanglement from realistic measurements, to, say, observe entanglement propagation [55]. Here again, notions of (quantitative) witnesses that provide bounds to entanglement measures play...
Using a quantum computer to efficiently perform computational tasks that are provably intractable for classical computers marks a key milestone in the development of quantum technologies. Various sub-universal models of quantum computing have been proposed to demonstrate, with near-term achievable technology, a so-called quantum advantage or quantum computational supremacy. A crucial part of the demonstration of this claim with a given model is the verification of the output of the corresponding quantum device. But the nature of the computational task is precisely such that it cannot be reproduced classically and therefore the traditional means of verifying a computation fail. What is more, the proposed sub-universal quantum devices produce samples from exponentially flat probability distributions to the effect that it requires exponentially many samples to classically verify that the obtained samples are indeed distributed according to the target distribution, independently of the hardness of producing the samples [47, 95]. The latter result severely restricts the possibilities for deriving classical verification protocols for quantum computational supremacy even under the assumption that the verifier has access to arbitrary computational power.

To circumvent this no-go result and arrive at a sample-efficient verification protocol one may take very different routes: First, one might ask for less than verification of the full output distribution such as merely distinguishing against the uniform or certain efficiently sampleable distributions, which can often be done in a computationally efficient way [2, 21, 76, 87]. Allowing for exponential time in classical post-processing, one can also sample-efficiently verify coarse-grained versions of the target distribution [16], make use of certain complexity-theoretic assumptions [3], or assumptions on the noise in the quantum device [15, 16, 32]. The latter allows one to use weaker measures, like the cross-entropy [15, 16] or variants thereof. If one gives qualitatively more power to the user, e.g., trusted single-qubit measurements [48, 75, 91], this even allows one to fully efficiently verify the prepared quantum state and thereby the sampled distribution. Finally, one may use more complicated, interactive protocols which require a universal quantum device, e.g., the one presented in Ref. [64], which relies on the post-quantum security of a certain computational task to classically delegate a universal computation. Given the importance of verifying a quantum advantage, it is a pressing challenge to derive fully efficient verification protocols which involve minimal assumptions. We expect that this will require custom-tailored techniques for the different available proposals.

An important role [6, 29, 44]. Such witnesses can be measured by exploiting randomness [19].

In case one has a good understanding of the physical mechanisms governing the device, it is often useful to build trust in the quantum device. This approach is particularly prominent in quantum simulation: Here, the idea is to certify a quantum device by validating its correct functioning in certain classically simulable regimes through comparison to classical simulations [17, 84, 93, 94]. In some instances, stronger statements can be made when invoking notions of self-validation [59] or cross-platform validation [30]. It is also common to certify the components of a device, for example, individual gates, and extend the trust obtained in this way to the full device, making the assumption that all sources of errors are already present for the individual components. In such approaches, it is assumed that no additional sources of errors arise when moving out of the strictly certifiable regime again.

An important drawback of most schemes discussed so far, however, is that they assume i.i.d. state preparations. This limitation can be overcome using quantum de Finetti arguments to obtain non-i.i.d. tomographic regions [23, 99] and distance certificates [91], the use of which has been optimized in various works for the case of graph states [66, 90] as well as for continuous variable states [22].

More severely still, in the standard setting a high level of trust in the measurement devices is required giving rise to a vicious cycle: After all, to calibrate the measurement devices in the first place, one requires quantum probe states which are well characterized, a task that requires well-calibrated measurement devices. This raises the question whether one can simultaneously learn about the quantum device and the quantum measurement apparatus in a self-consistent or semi-device-dependent way. The rather extreme and resource-intense solution to this problem is gate set tomography which instead of focusing on a single quantum channel or state, characterizes an entire set of quantum gates, the state preparation and the measurement self-consistently from different gate sequences [13, 14, 69]. Other solutions have been demonstrated in optics settings where one can perform state tomography in a self-calibrating way [18, 70]. Such schemes at times even come with error bars [86]. One can also exploit well characterized reference states such as coherent states [71] as a lever to perform uncalibrated tomography [79]. In another vein, one can mitigate uncertainty in the model that generated the data by using model averaging techniques [34]. A particularly important example of fidelity-estimation protocols for quantum processes that break this vicious cycle is given by randomized benchmarking [28, 31, 61, 62] (see BOX 2).

One could imagine, however, applications where even mild assumptions cannot be guaranteed. In such a scenario, one could utilize a range of cryptographic tool-kits to ensure that the above assumptions are indeed enforced. One prominent example of such setting is where one has to work in a black-box setting, i.e., with no assumptions made about the underlying devices. Remarkably, the non-local correlations demonstrated by quantum mechanics allow for certain entangled states and non-commuting measurements to be certified in this setting (up to local isometries) solely via the observed statistics [67]. This procedure of self-testing is typically achieved through the violation of a Bell inequality, with the paradigmatic example being the maximal violation of the CHSH inequality which self-tests non-commuting Pauli measurements made upon a maximally entangled pair of qubits. A substantial body of literature has extended these results in many directions, including generalisations to multi-partite entangled states [68] and approximate collections of maximally entangled qubit pairs [80] which have been made increasingly robust [72] (a recent and comprehensive review of self-testing
In the context of computation, the key idea of device-independent schemes is to hide the delegated computation from a remote black box server in such a way that the powerful server cannot retrieve any information about the computation without leaking to the client that a deviation has occurred. The use of the quantum twirling lemma or similar technique allows one to simplify the analysis under a general deviation (with no assumptions) to a simple (i.i.d.) case leading to efficient verified blind quantum computation schemes [24, 36, 80]. Guarantees of correctness have been achieved in this manner in various scenarios, giving different degrees of control to the user. These powerful verification schemes, while removing many trust assumptions and providing efficient protocols, remain only applicable to a remote verifier with limited quantum capacity, such as single qubit gates [36], or access to entangled servers [24, 80]. These last obstacles have recently been overcome by utilizing yet another cryptographic toolkit, this time from the classical domain. The usage of post-quantum secure collision-resistant hash functions has enabled a fully classical client to hide and verify the remote quantum computation [41, 64]. However, these new schemes come with a significant overhead on the server side, and they are no longer fully unconditionally secure, as they are based on a computational assumption, that is, the existence of classical problems that are computationally hard to solve even for a quantum computer [78]. We provide a case study of how different certification methods can be applied in the context of verifying a quantum computational advantage (BOX 3).

d. Outlook. In this Expert Recommendation, we have provided an overview of methods for certifying and benchmarking quantum devices as they are increasingly becoming of key importance in the emerging quantum technologies (for detailed, up-to-date information, see (BOX 4)). This review is meant to be an invitation to a growing field of research that combines sophisticated mathematical reasoning with a data-driven experimental mindset and that may well be a make-or-break topic for quantum technologies.

e. Acknowledgements. D. H. gratefully acknowledges discussions with D. Gross. J. E. acknowledges funding from the DFG (CRC 183, EI 519/9-1, EI 519/14-1, EI 519/15-1, MATH+), the BMWF (Q.Link.X), the BMWi (PlanQK), and the Templeton Foundation. N. W. acknowledges funding support from the European Unions Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 750905. This work has also received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No. 817482 (PASQuanS). E. K. and D. M. acknowledge funding from the ANR project ANR-13-BS04-0014 COMB, E. K. by the EP-SRC (EP/N003829/1).

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### Table 1: Examples of verification protocols

| Verification protocol | Information | Feasibility | Samples | Complexity | Measurements |
|-----------------------|-------------|-------------|---------|------------|--------------|
| Blind computing via Bell test [24] | Trace distance | Characterized random unitary | O(1/\epsilon^2) | O(1/\epsilon^2) | n/qubits, classical data |
| Blind quantum computing via Bell test [24] | Trace distance | Characterized random unitary | O(1/\epsilon^2) | O(1/\epsilon^2) | n/qubits, classical data |
| Graph state schemes [66] | Trace distance | Characterized random unitary | O(1/\epsilon^2) | O(1/\epsilon^2) | n/qubits, classical data |

Note: The table entries are placeholders and should be filled with actual data from the document. The table structure and formatting are designed to represent the data in a readable and organized manner.
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