Reliable Quantum State Tomography

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(Dated: November 7, 2012)

Quantum state tomography is the task of inferring the state of a quantum system by appropriate measurements. Since the frequency distributions of the outcomes of any finite number of measurements will generally deviate from their asymptotic limits, the estimates computed by standard methods do not in general coincide with the true state, and therefore have no operational significance unless their accuracy is defined in terms of error bounds. Here we show that quantum state tomography, together with an appropriate data analysis procedure, yields reliable and tight error bounds, specified in terms of confidence regions—a concept originating from classical statistics. Confidence regions are subsets of the state space in which the true state lies with high probability, independently of any prior assumption on the distribution of the possible states. Our method for computing confidence regions can be applied to arbitrary measurements including fully coherent ones; it is practical and particularly well suited for tomography on systems consisting of a small number of qubits, which are currently in the focus of interest in experimental quantum information science.

PACS numbers: 03.65.Wj, 02.50.-r, 03.67.-a

The state of a classical system can in principle be determined to arbitrary precision by applying a single measurement to it. Any imprecisions are due solely to inaccuracies of the measurement technique, but not of fundamental nature. This is different in quantum theory. It follows from Heisenberg’s uncertainty principle that measurements generally have a random component and that individual measurement outcomes only give limited information about the state of the system—even if an ideal measurement device is used. To illustrate this difference, it is useful to take an information-theoretic perspective. Assume, for instance, that we are presented with a two-level system about which we have no prior information except that it has been prepared in a pure state, and our task is to determine this state. If the system was classical, there are only two possible pure states, and one single bit of information is therefore sufficient for its full description. Furthermore, a single measurement of the system suffices to retrieve this bit. If the system was quantum, however, the situation becomes more interesting. A two-level quantum system (a qubit) admits a continuum of pure states that can, for example, be parameterized by a point on the Bloch sphere. To determine this point to a given accuracy \( \Delta \), at least \( \log_2(4/\Delta^2) \) bits of information are necessary \([45]\). Conversely, according to Holevo’s bound \([1]\), any measurement applied to a single qubit will provide us with at most one bit of information. And even if \( n \) identically prepared copies of the qubit were measured, at most \( \log_2(n+1) \) bits of information about their state can be obtained \([45]\). Hence the accuracy, \( \Delta \), to which the state can be determined always remains finite \( (\Delta \geq \frac{1}{\sqrt{n+1}}) \), necessitating the specification of error bars.

The impact that randomness in measurement data has on the accuracy of estimates has been studied extensively in statistics and, in particular, estimation theory \([2]\). The latter is concerned with the general problem of estimating the values of parameters from data that depend probabilistically on them. The data may be obtained from measurements on a quantum system with parameter-dependent state, as considered in quantum estimation theory \([3]\). Quantum state tomography can be seen as a special instance of quantum estimation, where one aims to estimate a set of parameters large enough to determine the system’s state completely \([4–10]\).

An obvious choice of parameters are the matrix elements of a density operator representation of the state. Due to the finite accuracy, however, the individual estimates for the matrix elements do not generally correspond to a valid density operator (for instance, the matrix may have negative eigenvalues). This problem is avoided with other techniques, such as maximum likelihood estimation (MLE) \([8, 11, 12]\), which has been widely used in experiments \([13–19]\), or Bayesian estimation \([3, 20, 25]\).

In MLE, an estimate for the error bars can be obtained from the width of the likelihood function, which is approximated by the Fisher information matrix \([10, 11, 26–29]\). In current experiments one also uses numerical plausibility tests known as “bootstrapping” or, more generally, “resampling” \([18, 30]\) in order to obtain bounds on the errors. However, despite being reasonable in many practical situations, these bounds are not known to have a well-defined operational interpretation and, in the case of the resampling method, may lead to an underestimate of the errors \([31]\).

In contrast, Bayesian methods can be used to calculate “credibility regions”, i.e., subsets of the state space in which the state is found with high probability. This probability, however, depends on the choice of a “prior”, corresponding to an assumption about the distribution of the states before the measurements (in particular, the assumption can not be justified by the experimental data). Furthermore, we remark that most known techniques are based on the assumption of independent and identical measurements (a notable exception is the one-qubit adaptive tomography analysis of \([32]\)). We refer to \([23]\) for a further discussion of currently used approaches to quantum state tomography, including pedagogical examples illustrating their limitations.

In this Letter we introduce a method to obtain confidence
regions, that is, regions in state space which contain the true state with high probability. A point in the region may then serve as estimate and the maximal distance of the point to the border of the region as error bar. Our method allows to analyse data obtained from arbitrary quantum measurements, including fully coherent ones. The method does not rely on any assumptions about the prior distribution of the states to be measured. This makes it highly robust so that it can, for instance, be applied in the context of quantum cryptography, where the states to be estimated are chosen adversarially.

The remainder of this Letter is organized as follows. We first describe a very general setup for tomography of quantum states prepared in a sequence of experiments, where we do not make the typical assumption that the states are independent and identically distributed (i.i.d.). We then show that, nevertheless, properties of the states can be inferred reliably using a suitable tomographic data analysis procedure (Theorem 1). In motivation and spirit, this result relates to recent research efforts on quantum de Finetti representations. We then specialise our setup to the case where, in principle, the experiments may be run an arbitrary number of times (while still only finitely many runs are used to generate data). This special case is (by the quantum de Finetti theorem) equivalent to an i.i.d. preparation of the states, thereby justifying the common i.i.d. assumption in data analysis. The theorem, applied to this special case, then results in a construction for confidence regions for quantum state tomography (Corollary 1).

**General Scenario.**—Consider a collection \( S_1, \ldots, S_{n+k} \) of finite-dimensional quantum systems with associated Hilbert space \( \mathcal{H} \), as depicted in Fig. 1 (see also [33] and [34], where a similar setup is considered). We denote by \( d \) the dimension of \( \mathcal{H} \). For example, one may think of \( n + k \) particles prepared in a series of experiments, where \( \mathcal{H} \) could correspond to the spin degree of freedom. From this collection, a sample consisting of \( n \) systems is selected at random and measured according to an (arbitrary) Positive Operator Valued Measure (POVM) \( \{ B^n \} \), a family of positive semi-definite operators \( B^n \) on \( \mathcal{H} \otimes \mathcal{N} \) such that \( \sum_{B^n} B^n = 1_{\mathcal{H} \otimes \mathcal{N}} \). That is, each POVM element \( B^n \) corresponds to a possible sequence of outcomes resulting from (not necessarily independent) measurements on the \( n \) systems. The goal of quantum state tomography is to infer the state of the remaining \( k \) systems, using the outcomes of these measurements.

Note that the \( k \) extra systems are not measured during data acquisition. Nevertheless, they play a role in the above scenario, as they are used to define operationally what state we are inferring. (In the special case of i.i.d. states, the extra systems are simply copies of the measured systems—see below.) We also remark that, instead of measuring a sample of \( n \) systems chosen at random, one may equivalently permute the initial collection of \( n + k \) systems at random and then measure the first \( n \) of them, i.e., \( S_1, \ldots, S_n \). We will use this alternative description for our theoretical analysis.

In order to describe our main results, we imagine that the measurement outcomes \( B^n \) are processed by a data analysis routine that outputs a probability distribution \( \mu_{B^n} \) on the set of mixed states, defined by

\[
\mu_{B^n}(\sigma)d\sigma = \frac{1}{c_{B^n}} \text{tr}[\sigma \otimes B^n]d\sigma
\]

(see Fig. 2 for an illustration). Here \( d\sigma \) denotes the Hilbert-Schmidt measure with \( \int d\sigma = 1 \). Furthermore, \( c_{B^n} = \text{tr}[B^n \otimes 1_{\mathcal{K}^n} \cdot 1_{\text{Sym}^n(\mathcal{H} \otimes \mathcal{K})}] \) is a normalisation constant, where \( \mathcal{K} \cong \mathcal{H} \cong \mathbb{C}^d \) and where \( 1_{\text{Sym}^n(\mathcal{H} \otimes \mathcal{K})} \) is the projector onto the symmetric subspace of \( (\mathcal{H} \otimes \mathcal{K})^n \). Note that, in Bayesian statistics, \( \mu_{B^n}(\sigma)d\sigma \) corresponds to the a posteriori distribution when updating a Hilbert-Schmidt prior \( d\sigma \). Furthermore, in MLE, \( \sigma \mapsto \text{tr}[\sigma \otimes B^n] \) is known as the likelihood function. Since our work is not based on either of these approaches, however, we will not use this terminology and simply refer to \( \mu_{B^n} \).

**Reliable Predictions.**—We now show that \( \mu_{B^n} \) contains all information that is necessary in order to make reliable predictions about the state of the remaining systems \( S_{n+1}, \ldots, S_{n+k} \). To specify these predictions, we consider hypothetical tests, a quantum version of a similar concept used in classical statistics. Any such test acts on the joint system consisting of \( S_{n+1}, \ldots, S_{n+k} \) (see Fig. 1). Mathematically,
The test is simply a measurement with binary outcome, “success” or “failure,” specified by a joint POVM \( \{ T_{\text{fail}}, 1_H^k - T_{\text{fail}} \} \) on \( \mathcal{H}^k \). Note that the state of \( S_{n+1}, \ldots, S_{n+k} \) could be inferred if we knew which hypothetical tests it would pass. Hence, instead of estimating this state directly, we can equivalently consider the task of predicting the outcomes of the hypothetical tests.

Assume now that we carry out a test \( T_{\mu_B^n} = \{ T_{\text{fail}}, 1_H^k - T_{\text{fail}} \} \) depending on \( \mu_B^n \). We denote by \( \rho_{n+k} \) the (unknown) joint state of the systems \( S_1, \ldots, S_{n+k} \) before the tomographic measurements. (As described above, we can assume without loss of generality that the systems are permuted at random, so that \( \rho_{n+k} \) is permutation invariant.) If the outcome of the tomographic measurement is \( B^n \), then the post-measurement state of the remaining systems is given explicitly by \( \rho_{B^n} = \frac{1}{\text{tr}[\rho_{B^n}]} \text{tr}_{\mathcal{H}^k}[B^n \otimes 1_H^k \cdot \rho_{n+k}] \), where \( \text{tr}_{\mathcal{H}^k} \) denotes the partial trace over the \( n \) measured systems. Hence, the probability that the test \( T_{\mu_B^n} \) fails for the above state \( \rho_{B^n} \) equals \( \text{tr}[T_{\text{fail}} \rho_{B^n}] \). The following theorem now provides a criterion under which this failure probability is upper bounded by any given \( \varepsilon > 0 \). Crucially, the criterion only depends on \( \mu_B^n \), which is obtained by the tomographic data analysis. In other words, \( \mu_B^n \) allows us to determine which hypothetical tests the state \( \rho_{B^n} \) would pass.

**Theorem 1** (Reliable Predictions from \( \mu_B^n \)). For all \( B^n \) let \( T_{\mu_B^n} \) be a POVM element on \( \mathcal{H}^k \) such that

\[
\int \mu_B^n(\sigma) \text{tr}[T_{\text{fail}} \rho_{\mu_B^n} \sigma] d\sigma \leq \varepsilon c_{n+k,d},
\]

where \( c_{N,d} = \binom{N+d-1}{d} \). Then, for any \( \rho_{n+k} \)

\[
\langle \text{tr}[T_{\text{fail}} \rho_{\mu_B^n} \rho^n] \rangle_{B^n} \leq \varepsilon,
\]

where \( \langle \cdot \rangle_{B^n} \) denotes the expectation taken over all possible measurement outcomes \( B^n \) when measuring \( \rho^n \) (i.e., outcome \( B^n \) has probability \( \text{tr}[B^n \rho^n] \)).

As we shall see, the tests are typically chosen such that the integral over \( d\sigma \) decreases exponentially with \( n \). The additional factor \( c_{n+k,d}^{-1} \), which is inverse polynomial in \( n+k \), plays therefore only a minor role in the criterion. We also emphasize that the theorem is valid independently of how the systems \( S_1, \ldots, S_{n+k} \) have been prepared. In particular, the (commonly made) assumption that they all contain identical copies of a single-system state is not necessary.

The proof of the theorem, together with a slightly more general formulation, is provided in the Supplemental Information. It makes crucial use of the following fact, which has also been used in quantum-cryptographic security proofs: there exists a so-called de Finetti state \( \tau^N \), i.e., a convex combination of tensor products, such that \( \rho^n \leq c_{N,d} \cdot \tau^N \) holds for all permutation-invariant states \( \rho^n \) on \( \mathcal{H}^N \).

**Confidence Regions.**—A confidence region is a subset of the single-particle state space which is likely to contain the “true” state. In order to formalize this, we consider the practically relevant case of an experiment that can in principle be repeated arbitrarily often. Within the above-described general scenario, this corresponds to the limit where \( k \) approaches infinity while \( n \), the number of actual runs of the experiment (whose data is analyzed), is still finite and may be small.

Since the initial state \( \rho_{n+k} \) of all \( n+k \) systems can without loss of generality be assumed to be permutation invariant (see above), the Quantum de Finetti Theorem \([33, 37–40]\) implies that, for fixed \( n, k' \in \mathbb{N} \), the marginal state \( \rho_{n+k'} \) on \( n+k' \) systems is approximated by a mixture of product states, i.e.,

\[
\rho_{n+k'} = \text{tr}_{k-k'}(\rho_{n+k}) \approx \int P(\sigma)\sigma^\otimes(n+k') d\sigma,
\]

for some probability density function \( P \) and approximation error proportional to \( 1/k \). In the limit of large \( k \), the marginal state \( \rho_{n+k'} \) is thus fully specified by \( P \). We can therefore equivalently imagine that all systems were prepared in the same unknown “true” state \( \sigma \), which is distributed according to \( P \) (see Fig. 3). This corresponds to the i.i.d. assumption commonly made in the literature on quantum state tomography, which is therefore rigorously justified within our general setup.

As before, we assume that tomographic measurements are applied to the systems \( S_1, \ldots, S_n \), whereas the remaining systems, \( S_{n+1}, \ldots, S_{n+k'} \), undergo a test (depending on the output \( \mu_B^n \) of the data analysis procedure). We may now consider tests that are passed if and only if the true state \( \sigma \) is contained in a given subset \( \Gamma_{\mu_B^n} \) of the state space. The following corollary provides a sufficient criterion under which the tests are passed, so that \( \Gamma_{\mu_B^n} \) are confidence regions. (Note that the criterion refers to additional sets \( \Gamma_{\mu_B^n} \) that are related to the confidence regions \( \Gamma_{\mu_B^n} \); see the Supplemental Information for an illustration.)

**Corollary 1** (Confidence Regions from \( \mu_B^n \)). For all \( B^n \) let

\[
\Gamma_{\mu_B^n}(\sigma) = \left\{ \rho^n : \text{tr}[T_{\text{fail}} \rho_{\mu_B^n} \sigma] \leq \varepsilon \right\},
\]

where \( \varepsilon > 0 \) is a parameter. Then, for any \( B^n \) and \( \sigma \in \mathcal{H}^k \),

\[
\langle \text{tr}[T_{\text{fail}} \rho^n \sigma] \rangle_{B^n} \leq \varepsilon,
\]

where \( \langle \cdot \rangle_{B^n} \) denotes the expectation taken over all possible measurement outcomes \( B^n \) when measuring \( \sigma \) (i.e., outcome \( B^n \) has probability \( \text{tr}[B^n \sigma] \)).
Note that $1 - \varepsilon$ can be interpreted as the confidence level of the statement that the true state $\sigma$ is contained in the set $\Gamma^\delta_{\mu B^n}$. Crucially, the claim is valid for all $\sigma$. In particular, it is independent of any initial probability distribution, $P$, according to which $\sigma$ may have been chosen (see Eq. (4)). In other words, the operational interpretation of the sets $\Gamma^\delta_{\mu B^n}$ as confidence regions does not depend on any extra assumptions about the preparation procedure or on the specification of a prior. In fact, $\sigma$ could even be chosen “maliciously”, for example in a quantum cryptographic context, where an adversary may try to pretend that a system has certain properties (e.g., that its state is entangled while in reality it is not).

Obviously, the assertion that a state $\sigma$ is contained in a certain set $\Gamma^\delta_{\mu}$ can only be considered a good approximation of $\sigma$ if the set $\Gamma^\delta_{\mu}$ is small. This is indeed the case for reasonable choices of the measurement $\{B^n\}$. For instance, in the practically important case where each system is measured independently and identically with POVM $\{E_i\}$, the confidence region is, for generic states, asymptotically of size proportional to $\frac{1}{\sqrt{n}}$ in the (semi-)norm on the set of quantum states induced by the POVM: $\|\cdot\|_{\{E_i\}} = \sum_i |\text{tr}(E_i \cdot)|$ (see Supplemental Information and [42]).

Conclusion.—Despite conceptual differences, our technique is not unrelated to MLE and Bayesian estimation. As mentioned before, $\mu(\sigma)$ is proportional to the likelihood function and, therefore, methods to construct confidence regions with our technique are likely to use adaptations of techniques from MLE. Also, $\mu_B^n(\sigma)d\sigma$ corresponds to the probability measure obtained from applying Bayes’ updating rule to the Hilbert-Schmidt measure; a fact that implies near optimality [48] of our method in the practically most relevant case of independent tomographically complete measurements [23].

Recently, another novel approach to quantum state tomography has been proposed [43,44], which yields reliable error bounds similar to ours. A central difference between this approach and ours is the level of generality. In [43,44] a specific sequence of measurement operations is proposed, which is adapted to systems whose states are fairly pure. Under this condition, the estimate converges fast and, in addition, can be computed efficiently. In contrast, our method can be applied to arbitrary measurements (i.e., any tomographic data may be analyzed). Accordingly, the convergence of the confidence region depends on the choice of these measurements. However, we do not propose any specific algorithm for the efficient computation of confidence regions.

Finally, we refer to the very recent work of Blume-Kohout [31] for an excellent discussion of the notion of confidence regions in quantum state tomography. In particular, he shows that confidence regions, as considered here, can be defined via likelihood ratios.

Acknowledgements.—We thank Robin Blume-Kohout for useful comments on earlier versions of this work. We acknowledge support from the Swiss National Science Foundation (grants PP00P2-128455 and 200020-135048, and through the National Centre of Competence in Research ‘Quantum

FIG. 3: Tomography of identically prepared systems. This scenario falls into the framework depicted in Fig.[1] corresponding to the limit where the number of extra systems, $k$, approaches infinity. In this case, we can assume without loss of generality that the systems have been prepared in a two-step process: first, a description “a” of a single-system state is sampled at random (according to some probability density $P$); second, $n$ identical systems $S_1, \ldots, S_n$ are prepared in state $\sigma$. The $k$ extra systems of Fig.[1] are replaced by a classical variable carrying the description “a”. Given only the output of the tomographic data analysis, $\mu_{B^n}$, it is possible to decide whether $\sigma$ is (with probability at least $1 - \varepsilon$) contained in a given set $\Gamma^\delta_{\mu_{B^n}}$ (Corollary 1). If this is the case then $\Gamma^\delta_{\mu_{B^n}}$ is a confidence region (with confidence level $1 - \varepsilon$).

Given $\mu_{B^n}$ be a set of states on $\mathcal{H}$ such that

$$\int_{\Gamma_{\mu B^n}} \mu_{B^n}(\sigma) d\sigma \geq 1 - \frac{\varepsilon}{2} c_{n,\beta}^{-1}.$$  (2)

Then, for any $\sigma$,

$$\text{Prob}_{B^n}[\sigma \in \Gamma^\delta_{\mu_{B^n}}] \geq 1 - \epsilon,$$

where $\text{Prob}_{B^n}$ refers to the distribution of the measurement outcomes $B^n$ when measuring $\sigma \otimes n$ (i.e., outcome $B^n$ has probability $\text{tr}(B^n \sigma \otimes n)$) and where

$$\Gamma^\delta_{\mu_{B^n}} = \{ \sigma : \exists \sigma' \in \Gamma_{\mu_{B^n}}, \text{with } F(\sigma, \sigma')^2 \geq 1 - \delta^2 \},$$  (3)

with $\delta^2 = \frac{2}{n} (\ln \frac{2}{\varepsilon} + 2 \ln c_{2n,\beta})$ and $F(\sigma, \sigma') = \| \sqrt{\sigma} \sqrt{\sigma'} \|_1$ the fidelity.

The main idea for the proof of the corollary is to apply the above theorem to tests (acting on $k' = n$ systems) derived from Holevo’s optimal covariant measurement [41]. We refer to the Supplemental Information for the technical proof.
Science and Technology’), the German Science Foundation (grant CH 843/2-1), and the European Research Council (grant 258932).

[1] A. Holevo, Probl. Peredachi Inf. 9, 31 (1973).
[2] S. Kay, Fundamentals of Statistical Signal Processing: Estimation Theory, vol. 1 (Prentice Hall, 1993).
[3] C. W. Helstrom, Quantum Detection and Estimation Theory (Academic Press, New York, 1976).
[4] U. Fano, Rev. Mod. Phys. 29, 74 (1957).
[5] K. Vogel and H. Risken, Phys. Rev. A 40, 2847 (1989).
[6] D. T. Smithey, M. Beck, M. G. Raymer, and A. Faridani, Phys. Rev. Lett. 70, 1244 (1993).
[7] U. Leonhardt, H. Paul, and G. M. D’Ariano, Phys. Rev. A 52, 4899 (1995).
[8] Z. Hradil, Phys. Rev. A 55, R1561 (1997).
[9] G. M. D’Ariano, M. G. Paris, and M. F. Sacchi, in Advances in Imaging and Electron Physics, edited by P. W. Hawkes (Elsevier, 2003), vol. 128, pp. 205 – 308.
[10] T. Sugiyama, P. S. Turner, and M. Murao, Phys. Rev. A 83, 012105 (2011).
[11] K. Banaszek, G. M. D’Ariano, M. G. A. Paris, and M. F. Sacchi, Phys. Rev. A 61, 010304 (1999).
[12] Z. Hradil, J. Řeháček, J. Fiurášek, and M. Ježek, in Quantum State Estimation, edited by M. Paris and J. Řeháček (Springer, 2004), pp. 59–112.
[13] D. F. V. James, P. G. Kwiat, W. J. Munro, and A. G. White, Phys. Rev. A 64, 052312 (2001).
[14] C. F. Roos, G. P. T. Lancaster, M. Riebe, H. Häffner, W. Hänsel, S. Gulde, C. Becher, J. Eschner, F. Schmidt-Kaler, and R. Blatt, Phys. Rev. Lett. 92, 220402 (2004).
[15] J. K. Resch, P. Walther, and A. Zeilinger, Phys. Rev. Lett. 94, 070402 (2005).
[16] R. Blatt and D. Wineland, Nature 453, 1008 (2008).
[17] S. Filipp, P. Maurer, P. J. Leek, M. Baur, R. Bianchetti, J. M. Fink, M. Göppi, L. Steffen, J. M. Gambetta, A. Blais, et al., Phys. Rev. Lett. 102, 200402 (2009).
[18] J. P. Home, D. Hanneke, J. D. Jost, J. M. Amini, D. Leibfried, and D. J. Wineland, Science 325, 1227 (2009).
[19] J. T. Barreiro, M. Müller, P. Schindler, D. Nigg, T. Monz, M. Chwalla, M. Hennrich, C. F. Roos, P. Zoller, and R. Blatt, Nature 470, 486 (2011).
[20] K. R. W. Jones, Ann. Phys. (NY) 207, 140 (1991), ISSN 0003-4916.
[21] V. Bužek, R. Derka, G. Adam, and P. Knight, Ann. Phys. (NY) 266, 454 (1998).
[22] R. Schack, T. A. Brun, and C. M. Caves, Phys. Rev. A 64, 014305 (2001).
[23] F. Tanaka and F. Komaki, Phys. Rev. A 71, 052323 (2005).
[24] R. Blume-Kohout, New J. Phys. 12, 043034 (2010).
[25] K. Audenaert and S. Scheel, New J. Phys. 11, 023028 (2009).
[26] K. Usami, Y. Nambu, Y. Tsuda, K. Matsumoto, and K. Nakamura, Phys. Rev. A 68, 022314 (2003).
[27] Z. Hradil, D. Mogilevtsev, and J. Řeháček, Phys. Rev. Lett. 96, 230401 (2006).
[28] M. D. de Burgh, N. K. Langford, A. C. Doherty, and A. Gilchrist, Phys. Rev. A 78, 052122 (2008).
[29] J. Řeháček, D. Mogilevtsev, and Z. Hradil, New J. Phys. 10, 043022 (2008).
[30] R. J. T. B. Efron, An Introduction to the Bootstrap (Chapman & Hall, 1993).
[31] R. Blume-Kohout (2012), arXiv:1202.5270.
[32] T. Sugiyama, P. S. Turner, and M. Murao, Phys. Rev. A 85, 052107 (2012).
[33] R. Renner, Nature Phys. 3, 645 (2007).
[34] G. Chiribella, in Theory of Quantum Computation, Communication, and Cryptography, edited by W. van Dam, V. Kendon, and S. Severini (Springer Berlin / Heidelberg, 2011), vol. 6519 of Lecture Notes in Computer Science, pp. 9–25.
[35] M. Hayashi, Comm. Math. Phys. 293, 171 (2010).
[36] M. Christandl, R. König, and R. Renner, Phys. Rev. Lett. 102, 020504 (2009).
[37] R. L. Hudson and G. R. Moody, Z. Wahrscheinv. verw. Geb. 33, 343 (1976).
[38] G. A. Raggio and R. F. Werner, Helv. Phys. Acta 62, 980 (1989).
[39] C. M. Caves, C. A. Fuchs, and R. Schack, J. Math. Phys. 43, 4537 (2002).
[40] M. Christandl, R. König, G. Mitchison, and R. Renner, Comm. Math. Phys. 273, 473 (2007).
[41] A. Holevo, Probabilistic and Statistical Aspects of Quantum Theory (North-Holland, Amsterdam, 1982).
[42] W. Matthews, S. Wehner, and A. Winter, Comm. Math. Phys. 291, 813 (2009).
[43] D. Gross, Y.-K. Liu, S. T. Flammia, S. Becker, and J. Eisert, Phys. Rev. Lett. 105, 150401 (2010).
[44] M. Cramer, M. B. Plenio, S. Flammia, D. Gross, S. Bartlett, R. Somma, O. Landon-Cardinal, Y.-K. Liu, and D. Poulin, Nature Comm. 1, 149 (2010).
[45] A disc with (great-circle) radius $\Delta$ on the Bloch sphere has area $2\pi(1 - \cos \Delta) \leq \pi \Delta^2$, whereas the full Bloch sphere has area $4\pi$. Consequently, there are at least $(4\pi)/(\pi \Delta^2) = 4/\Delta^2$ such discs. Note also that the (great-circle) distance $\Delta$ between two pure states $\phi$ and $\psi$ is related to their fidelity, $F(\phi, \psi) = \langle \phi | \psi \rangle = \cos \frac{\Delta}{2}$, as well as to their trace distance, $d(\phi, \psi) = 2 |\langle \phi | \psi \rangle| = 2 |\sin \frac{\Delta}{2}| \approx \Delta$.
[46] The bound follows from the fact that the joint state of $n$ identically prepared copies of a pure state in $\mathcal{H} = \mathbb{C}^2$ lies in the symmetric subspace of $\mathcal{H}^\otimes n$, which has dimension $n + 1$.
[47] For our technical treatment (see Supplemental Information), we also consider tests that act on a larger space, $(\mathcal{H} \otimes \mathcal{K})^\otimes k$, which includes purifications of the systems.
[48] More precisely, the bound on the parameter $\varepsilon$, which is usually exponentially decreasing in the size of the confidence region $\Gamma_{\varepsilon, \infty}$, is tight up to a polynomial factor.
Supplemental Information

Note: This document contains additional material (Appendices A, B, C, and D) that is not included in the “Supplemental Information” accompanying the journal version.

In the first part, we give precise statements and proofs of our technical results (Section 1), discuss the practically important case of independent measurements (Section 2) and present further remarks (Section 3). The second part explains how to represent states on the symmetric subspace (Appendix A) as well as functions on the state space (Appendices B and C), and concludes with examples (Appendix D).

1 Statements and Proofs

Let $\mathcal{H}$ be a Hilbert space of finite dimension $d$, i.e., $\mathcal{H} \cong \mathbb{C}^d$. We denote the set density matrices on $\mathcal{H}$ by $S(\mathcal{H})$ and the subset of pure states by $\mathcal{P}(\mathcal{H})$. Note that $\mathcal{P}(\mathcal{H})$ can be identified with $\mathbb{C}P^{d-1}$, the complex projective space of dimension $d-1$. $\mathbb{C}P^{d-1}$ carries a natural action of the unitary group $U(d)$. The Haar measure on $U(d)$ therefore descends to a measure on $\mathcal{P}(\mathcal{H})$ which is invariant under the action of $U(d)$. We denote this measure by $d\phi$ and fix the normalisation so that $\int d\phi = 1$. The symmetric subspace $\text{Sym}^n(\mathcal{H})$ of $\mathcal{H}^\otimes n$ is defined as the space of vectors that are invariant under the action of the symmetric group $S_n$ that permutes the tensor factors. Since the action of $S_n$ commutes with the action of the unitary group on $\mathcal{H}^\otimes n$, $U(d)$ acts on $\text{Sym}^n(\mathcal{H})$ as well. We denote the dimension of $\text{Sym}^n(\mathcal{H})$ by $\dim(n, d)$. The following lemma [1][2] is crucial in the derivation of the main results.

**Lemma 1.** Let $\rho^n \in S(\text{Sym}^n(\mathbb{C}^d))$. Then

$$\rho^n \leq \dim(n, d) \int \phi^\otimes n d\phi.$$  

**Further more, $\dim(n, d) = \frac{(n+d-1)}{n} \leq (n+1)^{d-1}$.**

The state defined by the integral on the right hand side is sometimes called de Finetti state. Note that the corresponding statement mentioned in the Letter for general permutation-invariant density operators $\rho^n$ is obtained from this lemma by considering a purification of $\rho^n$ in the symmetric subspace (see [2]).

**Proof.** The space $\text{Sym}^n(\mathbb{C}^d)$ is irreducible under the action of the unitary group $U(d)$ [3]. The operator $\int \phi^\otimes n d\phi$ is supported on $\text{Sym}^n(\mathbb{C}^d)$ and invariant under the action of $U(d)$. By Schur’s lemma we therefore have

$$\dim(n, d) \int \phi^\otimes n d\phi = 1_{\text{Sym}^n(\mathbb{C}^d)}.$$  

The claim follows since

$$\rho^n \leq 1_{\text{Sym}^n(\mathbb{C}^d)}$$

holds for any density operator. $\dim(n, d)$ equals $\binom{n+d-1}{n}$ and is easily seen to be upper bounded by $(n+1)^{d-1} = \text{poly}(n)$.

Consider now the measure $d\phi$ on a tensor product space $\mathcal{H} \otimes \mathcal{K}$, where $\mathcal{K} \cong \mathcal{H} \cong \mathbb{C}^d$ and perform the partial trace operation over system $\mathcal{K}$. We denote the resulting measure by $d\sigma$ on $S(\mathcal{H})$ and note that it may also be defined as the measure induced by the Hilbert-Schmidt metric [4]. (In the Letter, we refer to $d\sigma$ as the Hilbert-Schmidt measure.) For any POVM element $B^n$ on $\mathcal{H}^\otimes n$, our data analysis procedure produces a probability distribution

$$\mu_{B^n}(\sigma)d\sigma := \frac{1}{c_{B^n}} \text{tr}[B^n \sigma^\otimes n]d\sigma,$$

where $c_{B^n} = \int \text{tr}[B^n \sigma^\otimes n]d\sigma = \text{tr}[B^n \otimes 1_{\mathcal{K}^n} \cdot 1_{\text{Sym}^n(\mathcal{H} \otimes \mathcal{K})}]$. Let $\rho^{n+k}$ be a permutation-invariant density operator on $\mathcal{H}^\otimes n+k$ and $\varrho^{n+k}$ a purification with support on $\text{Sym}^{n+k}(\mathcal{H} \otimes \mathcal{K})$ (see e.g. [5]). That is, $\varrho^{n+k}$ is pure and $\text{tr}_{\mathcal{H}^\otimes n} \varrho^{n+k} = \rho^{n+k}$. Denote by $\varrho^{n+k}_{B^n} := \frac{1}{c_{B^n}} \text{tr}_{\mathcal{K}^n}[B^n \otimes 1_{\mathcal{K}^n} \cdot 1_{\text{Sym}^n(\mathcal{H} \otimes \mathcal{K})} \cdot \varrho^{n+k}]$ the post-measurement state and note that it appears with probability $\text{tr}[B^n \rho^n]$. Furthermore, we define $\nu_{B^n}(x) := \frac{1}{c_{B^n}} \text{tr}[B^n \otimes 1_{\mathcal{K}^n} \cdot |x\rangle\langle x|^\otimes n]$ for $x \in \mathcal{H} \otimes \mathcal{K}$. The following theorem holds for any POVM element $T_{\mu_{B^n}}$ on $(\mathcal{H} \otimes \mathcal{K})^\otimes k$. 
The failure probability of the test is given by
\[ \int \nu_{B^n}(x) \text{tr}[T_{\mu_{B^n}}^\text{fail} \rho_{\overline{B^n}}]dx \leq \varepsilon \left( \frac{n + k + d^2 - 1}{d^2 - 1} \right)^{-1}, \] (4)
then
\[ \langle \text{tr}[T_{\mu_{B^n}}^\text{fail} \rho_{B^n}] \rangle_{B^n} \leq \varepsilon, \]
where \( \langle \cdot \rangle_{B^n} \) denotes the expectation taken over all possible measurement outcomes \( B^n \) according to the probability distribution \( \text{tr}[B^n \rho^n] \).

Note that the probability distribution \( \mu_{B^n}(\sigma)d\sigma \) is obtained from the probability distribution \( \nu_{B^n}(x)dx \) by taking the partial trace over the purifying system \( K \). The above theorem therefore immediately implies the theorem in the Letter, which corresponds to the specialisation where \( T_{\mu_{B^n}}^\text{fail} \) acts only on \( \mathcal{H} \otimes k \).

**Proof.**

\[ \langle \text{tr}[T_{\mu_{B^n}}^\text{fail} \rho_{B^n}] \rangle_{B^n} = \sum_{B^n} \text{tr}[(B^n \otimes 1^n_k) \otimes T_{\mu_{B^n}}^\text{fail} \cdot \rho^{n+k}] \leq \dim(n + k, d^2) \sum_{B^n} \text{tr}[(B^n \otimes 1^n_k) \otimes T_{\mu_{B^n}}^\text{fail} \cdot |x\rangle\langle x|^{\otimes n+k}]dx \]
\[ = \dim(n + k, d^2) \sum_{B^n} c_{B^n} \int \nu_{B^n}(x) \text{tr}[T_{\mu_{B^n}}^\text{fail} |x\rangle\langle x|^{\otimes k}]dx \leq \varepsilon, \]
where we used Lemma \[ \Box \] in the first inequality and the assumption, \[ \Box \], in the second. \( \Box \)

For a subset \( \Gamma_\mu \) of \( S(\mathcal{H}) \), we define
\[ \Gamma_\mu^\delta = \{ \sigma : \exists \sigma' \in \Gamma_\mu \text{ with } P(\sigma, \sigma') \leq \delta \}, \]
where \( P(\sigma, \sigma') \) is the purified distance defined as \( \sqrt{1 - F(\sigma, \sigma')^2} \), where \( F(\sigma, \sigma') = \| \sqrt{\sigma} \sqrt{\sigma'} \|_1 = \text{tr} \sqrt{\sigma} \sqrt{\sigma'} \) is the fidelity. For more details regarding the purified distance as well as its relation to the trace distance see [6].

**Corollary 1** (Confidence Regions from \( \mu_{B^n} \)). For all \( B^n \), let \( \Gamma_{\mu_{B^n}} \) be such that
\[ \int_{\Gamma_{\mu_{B^n}}} \mu_{B^n}(\sigma)d\sigma \geq 1 - \frac{\varepsilon}{2} \left( \frac{2n + d^2 - 1}{d^2 - 1} \right)^{-1}, \] (5)
and let \( \delta := \sqrt{\frac{2}{n} \left( \ln \frac{2}{\varepsilon} + 2 \ln \left( \frac{2n + d^2 - 1}{d^2 - 1} \right) \right)} \). Then for all \( \sigma \),
\[ \text{Prob}_{B^n}[\sigma \in \Gamma_{\mu_{B^n}}^\delta] \geq 1 - \varepsilon \]
where the probability is with respect to the measurement outcomes \( B^n \) according to the probability distribution \( \text{tr}[B^n \sigma^{\otimes n}] \).

See Figure \[ \Box \] for an illustration of \( \Gamma_{\mu_{B^n}}^\delta \) and its relation to \( \mu_{B^n} \).

**Proof.** The failure probability of the test is given by
\[ P_{\text{fail}}(P) := \int P(\sigma) \sum_{B^n} \text{tr}[B^n \cdot \sigma^{\otimes n}] \Theta_{\Gamma_{\mu_{B^n}}}^\delta(\sigma)d\sigma \]
where \( \Theta_{\Gamma_{\mu_{B^n}}}^\delta(\sigma) \) equals one for \( \sigma \) in the set \( \Gamma_{\mu_{B^n}}^\delta \) and zero otherwise (\( \overline{A} \) denotes the complement of a subset \( A \) of \( S(\mathcal{H}) \)). This can be rewritten more conveniently as
\[ P_{\text{fail}}(P) = \sum_{B^n} c_{B^n} \int_{\Gamma_{\mu_{B^n}}} P(\sigma) \mu_{B^n}(\sigma)d\sigma. \]
FIG. 4: Construction of the confidence region. The graph schematically illustrates a possible distribution $\mu \equiv \mu_{B^n}$ (blue line), a high probability set $\Gamma_\mu$ of $\mu$ (blue bar), and the set $\Gamma_\mu^\delta$ which includes a $\delta$-region around $\Gamma_\mu$ (orange bar). In the scenario depicted by Fig. 3 in the Letter, the state $\sigma$ chosen by the preparation procedure is with high probability (at least $1 - \varepsilon$) in $\Gamma_\mu^\delta$, which can therefore be seen as a confidence region.

Instead of the a priori probability density $P(\sigma)$ we consider a probability density $Q(\psi)$ on the pure states $\mathcal{P}(\mathcal{H} \otimes \mathcal{K})$, where $\mathcal{K} \cong \mathcal{H}$, that gives rise to $P(\sigma)$. That is, $Q(\psi)$ satisfies

$$\int_A P(\sigma)d\sigma = \int_{\psi:\text{tr}_K\psi \in A} Q(\psi)d\psi$$

for all measurable subsets $A$ of $\mathcal{S}(\mathcal{H})$. Note that such a probability density $Q(\psi)$ always exists as we can purify the state of the particle with a purifying space $\mathcal{K} \cong \mathcal{H}$. $\mu_{B^n}(\sigma)$ is replaced by

$$\nu_{B^n}(\psi) := \frac{1}{c_{B^n}} \text{tr}[\{B^n \otimes \mathbb{I}_{\mathcal{K}}^{\otimes n}\cdot \psi^{\otimes n}\}].$$

Furthermore we consider the following extension of the set $\Gamma_\mu$:

$$\Omega_\mu = \{\psi \in \mathcal{P}(\mathcal{H} \otimes \mathcal{K}) : \text{tr}_K\psi \in \Gamma_\mu\}$$

and of $\Gamma_\mu^\delta$:

$$\Omega_\mu^\delta = \{\psi \in \mathcal{P}(\mathcal{H} \otimes \mathcal{K}) : \text{tr}_K\psi \in \Gamma_\mu^\delta\}.$$

The failure probability of the test can then be expressed as

$$P_{\text{fail}}(P) = \sum_{B^n} c_{B^n} \int_{\Omega_{B^n}}^\Omega_{B^n^\delta} Q(\psi)\nu_{B^n}(\psi)d\psi.$$  \hspace{1cm} (6)

Let $k' \in \mathbb{N}$ be the number of systems that we use to approximate the test by a test procedure that is given by a POVM $\{T_{\text{fail}}, 1 - T_{\text{fail}}\}$. Defining

$$T_{\text{fail}}^{k'} := \text{dim}(k', \Delta^2) \int_{\Omega_{B^n}}^\Omega_{B^n^\delta} \phi^{\otimes k'}d\phi.$$
we see that for all $\psi \in \Omega_\mu$

$$\text{tr}T_{\Omega_\mu^{k'}}^\text{fail} = 1 - \text{dim}(k', d^2) \int_{\Omega_\mu^{k'}} \text{tr}([\phi \otimes k', \psi \otimes k']) d\phi$$

$$\geq 1 - \text{dim}(k', d^2) \max_{\phi \in \Omega_\mu^{k'}} F(\text{tr}_\mu \phi, \text{tr}_\mu \psi)^{k'}$$

$$\geq 1 - \text{dim}(k', d^2) e^{-\frac{\epsilon'^2}{2} k'}.$$

Inserting this estimate into (6) leads to

$$P_{\text{fail}}(P) \leq \sum_{B^n} c_{B^n} \int_{\Omega_{\mu B^n}} Q(\psi) \nu_{B^n}(\psi) (\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k']) + \epsilon'' d\psi.$$  

We now remove the restriction in the integral, thereby further weakening the estimate and obtain

$$P_{\text{fail}}(P) \leq \epsilon'' + \sum_{B^n} c_{B^n} \int Q(\psi) \nu_{B^n}(\psi) (\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k']) d\psi,$$

$$= \epsilon'' + \sum_{B^n} \int Q(\psi) \nu_{B^n}(\psi) (\text{tr}[(B^n \otimes 1^\otimes k') \otimes \psi \otimes k'] d\psi,$$

$$= \epsilon'' + \sum_{B^n} \text{tr}[(B^n \otimes 1^\otimes k') \otimes T_{\Omega_\mu B^n}^\text{fail} \cdot (\int Q(\psi) \psi \otimes n+k' d\psi)].$$

Applying Lemma 1 to the state $\int Q(\psi) \psi \otimes n+k' d\psi$ we can find an upper bound on this quantity which is independent of the initial distribution $P(\sigma)$ (or $Q(\psi)$):

$$P_{\text{fail}}(P) \leq \epsilon'' + \text{dim}(n+k', d^2) \sum_{B^n} \nu_{B^n}(\psi) (\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k']) d\psi,$$

$$= \epsilon'' + \text{dim}(n+k', d^2) \sum_{B^n} c_{B^n} \int_{\Omega_{\mu B^n}} \nu_{B^n}(\psi) (\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k']) d\psi,$$

$$+ \text{dim}(n+k', d^2) \sum_{B^n} c_{B^n} \int_{\Omega_{\mu B^n}} \nu_{B^n}(\psi) (\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k']) d\psi.$$ 

Since for $\psi \in \Omega_{\mu B^n}$

$$\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k'] \leq \text{dim}(k', d^2) \max_{\phi \in \Omega_\mu B^n} F(\text{tr}_\mu \phi, \text{tr}_\mu \psi)^{k'} \leq \text{dim}(k', d^2) e^{-\frac{\epsilon'^2}{2} k'} = \epsilon''$$

and since

$$\text{tr}[T_{\Omega_\mu B^n}^\text{fail} \cdot \psi \otimes k'] \leq 1$$

we find

$$P_{\text{fail}}(P) \leq \epsilon'' + \text{dim}(n+k', d^2) \epsilon'' + \text{dim}(n+k', d^2) \sum_{B^n} c_{B^n} \int_{\Omega_{\mu B^n}} \nu_{B^n}(\psi) d\psi,$$

$$= \epsilon'' + \text{dim}(n+k', d^2) \epsilon'' + \text{dim}(n+k', d^2) \sum_{B^n} c_{B^n} \int_{\Omega_{\mu B^n}} \nu_{B^n}(\sigma) d\sigma.$$  

We now set $k' = n$ and use the assumption

$$\int_{\Omega_{\mu B^n}} \nu_{B^n}(\sigma) d\sigma \geq 1 - \frac{\epsilon}{2} \text{dim}(2n, d^2)^{-1}.$$
for all \( \mu_{B^n} \). This results in

\[
P_{\text{fail}}(P) \leq \varepsilon'' + \dim(2n, d^2)\varepsilon'' + \frac{\varepsilon}{2} \leq \dim(2n, d^2)^2 e^{-\frac{\nu^2}{2}} + \frac{\varepsilon}{2}.
\]

Choosing \( \delta = \sqrt{\frac{2}{n} (\ln \frac{2}{\varepsilon} + 2 \ln \dim(2n, d^2))} \) ensures that

\[
P_{\text{fail}}(P) \leq \varepsilon.
\]

Inserting for \( P \) a Dirac delta distribution concludes the proof. \( \square \)

2 Independent Measurements

We now restrict our discussion to the case where \( B^n \) is of product form, i.e.

\[
B^n = \prod_{i=1}^{r} E_i \otimes f(i)
\]

where \( E_i \) are the elements of a POVM, i.e., \( E_i \geq 0 \) and \( \sum_{i} E_i = 1 \). \( f = (f(1), \ldots, f(r)) \) is the vector containing the frequencies with which the outcomes occur, i.e. \( f(i) \in \mathbb{N} \) and \( \sum_{i=1}^{n} f(i) = n \). We find

\[
\mu_{B^n}(\sigma) = \frac{1}{c_{B^n}} \prod_{i=1}^{r} (\text{tr} E_i \sigma)^{f(i)},
\]

where \( c_{B^n} = \int \text{tr} B^n \sigma \otimes \sigma \, d\sigma \). We now want to investigate the maximum of this function which we assume for simplicity to be unique, i.e. we assume that the POVM is tomographically complete. Since the log function is monotonically increasing, the \( \sigma \) which maximises this function can also be expressed as

\[
\sigma_{\text{max}} := \arg\max_{\sigma} (\sum_{i} f(i) \log \text{tr} E_i \sigma), \quad (7)
\]

where \( \bar{f}(i) = \frac{f(i)}{n} \) are the relative frequencies. This shows that the value at which \( \mu_{B^n} \) is maximised coincides with the density matrix that the Maximum Likelihood Estimation method infers since \( \sum_{i} f(i) \log \text{tr} E_i \sigma \) is the so-called “log likelihood function” \([7, \text{Eqs. (2) and (3)}]\).

The MLE method is therefore consistent with our method and our work can be seen as a theoretical justification of it. We emphasize that in contrast to MLE, our work shows how to compute reliable error bars. This implies in particular that most of the likely states (i.e. the states within the error bars) are not on the boundary of the state space, even though the maximum might lie on the boundary. Our method can therefore be seen as a resolution of the “problem” that the states predicted by MLE are unphysical because they lie on the boundary.

We now want to study the decay of \( \mu_{B^n} \) around its maxima. In general this is not easy, as the maxima might lie on the boundary of the set. Useful statements can be made however, when the maxima are in the interior of the set of states. We consider the decay exponent (i.e. \( \frac{1}{n} \) times the natural logarithm) of the function \( \text{tr} B^n \sigma \otimes \sigma \) which is

\[
-\sum_{i} \bar{f}(i) \ln \text{tr} E_i \sigma. \quad (8)
\]

We then search for the extreme points of the function

\[
-\sum_{i} \bar{f}(i) \ln \text{tr} E_i \sigma + c(\text{tr} \sigma - 1)
\]

where we introduced the Lagrange multiplier \( c \) in order to take care of the normalisation of the density matrix. The extreme points are characterised by the equations

\[
-\sum_{i} \bar{f}(i) \frac{E_i}{\text{tr} E_i \sigma} = c 1
\]
\[ \text{tr} \sigma = 1. \]

Let us for simplicity restrict to the case, where the \( E_i \) are linearly independent, then, since the \( E_i \) form a POVM, we have
\[ \bar{f}^{(i)} = \text{tr} E_i \sigma \]
as a condition for an extreme point.

In order to carry over these findings to the estimate density, we need to understand the behaviour of the normalisation constant \( c_{B_n} = \int \text{tr} B^n \sigma \otimes^n d\sigma \). Since
\[ \int \text{tr} B^n \sigma \otimes^n d\sigma \leq \max \sigma \text{tr} B^n \sigma \otimes^n \]
and by Lemma 1
\[ \int \text{tr} B^n \sigma \otimes^n d\sigma \geq \frac{1}{\text{poly}(n)} \max \sigma \text{tr} B^n \sigma \otimes^n \]
we find that \( \frac{1}{n} \ln c_{B_n} \) approaches the maximum of \( (9) \), \( - \sum_i \bar{f}^{(i)} \ln \bar{f}^{(i)} \), for large \( n \). The decay exponent, \( - \frac{1}{n} \ln \mu_{B^n} \), is therefore asymptotically equal to the relative entropy (in units of the natural logarithm)
\[ D(\bar{f} \| E(\sigma)) = \sum_i \bar{f}^{(i)} (\ln \bar{f}^{(i)} - \ln \text{tr} E_i \sigma) \]
where \( E(\sigma) = (\text{tr} E_1 \sigma, \ldots, \text{tr} E_r \sigma) \) (this shows in particular that the extreme points are maxima since the relative entropy is nonnegative). Pinsker’s inequality
\[ D(\bar{f} \| E(\sigma)) \geq \frac{1}{2} \| \bar{f} - E(\sigma) \|^2_1. \]
implies that the error bars around the maxima are therefore given by
\[ \epsilon = O \left( \frac{1}{\sqrt{n}} \right) \]
in the distance on the set of density matrices induced by the norm \( \| X \| := \| E(X) \|_1 = \sum_i |\text{tr} E_i X| \).

### 3 Remarks

We remark that it is possible to adapt our method to the case where additional information, e.g., about the rank of the state or its symmetry, is available, and thereby to establish confidence regions also in these situations. For example, if it is known that the state \( \rho^{n+k} \) is invariant under local actions (on the individual systems \( \mathcal{H} \)) of unitaries from a given set \( \mathcal{U} \), then the integral in (5) can be restricted to a subset \( \mathcal{S} \) of states \( \sigma \) on \( \mathcal{H} \) such that \( U \sigma U^\dagger = \sigma \) for any \( U \in \mathcal{U} \). Accordingly, the confidence region is given by \( \mathcal{S} \cap \Gamma_{\mu_{B^n}} \), provided the criterion of the corollary is satisfied.

We also note that the output of the data analysis, \( \mu_{B^n} \), can be specified using a representation in terms of generalised spherical harmonics. Data obtained from measurements on \( n \) systems specify exactly the moments of degree less than \( n \) of this representation. In particular, these moments contain all information that is needed for a later update of \( \mu_{B^n} \) based on additional measurement data (see Appendices). While in the case of i.i.d. measurements (with a finite number of outcomes) this representation of the measurement data is costly (\( O(\text{poly}(n)) \) bits) when compared to simply storing the frequencies (\( O(\log n) \) bits), it may be useful in the case of non-i.i.d. measurements or measurements with an unbounded (or even continuous) set of outcomes, since it does not depend on the number of outcomes.

### A Quasi-Probability Distributions

In this section we derive quasi-probability distribution representations for operators on \( \text{Sym}^n(\mathbb{C}^d) \) similar to the P- and Q-representations that are well-known from quantum optics.
Theorem 2 (Q-representation). Let $B$ be an operator on $\text{Sym}^n(\mathbb{C}^d)$. Then $B$ is uniquely determined by its $Q$-representation, the function

$$Q_B(x) = \langle x|^{\otimes n}B|x\rangle^{\otimes n},$$

where $|x\rangle = \sum_i x_i |i\rangle$, $x = (x_1, \ldots, x_d)^T \in \mathbb{C}^d$ and $\sum_i |x_i|^2 = 1$. When convenient we will view $Q$ as a function on $\mathbb{C}P^{d-1}$.

Proof. We adopt an argument very similar to the one used in [9, p. 30] in the context of Glauber coherent states. Note that the values

$$\langle x|^{\otimes n}B|x\rangle^{\otimes n}$$

for $x \in \mathbb{C}^d$ are determined by $\langle x|^{\otimes n}B|x\rangle^{\otimes n}$ for $x \in \mathbb{C}^d$ with $\sum_i |x_i|^2 = 1$. It therefore suffices to show that the values $\langle x|^{\otimes n}B|x\rangle^{\otimes n}$, $x \in \mathbb{C}^d$ determine $\langle x|^{\otimes n}B|x\rangle^{\otimes n}$, $x, x' \in \mathbb{C}^d$ uniquely. Let $\{|m\rangle\}$ be the Gelfand-Zetlin basis for $\text{Sym}^n(\mathbb{C}^d)$ (see Appendix B) and write

$$B = \sum_{m, m'} B_{m, m'}|m\rangle\langle m'|.$$ 

The function $\langle m'|x'\rangle^{\otimes n}$ is a polynomial in $x' \in \mathbb{C}^d$ and $\langle x|^{\otimes n}|m\rangle$ is a polynomial in $\bar{x}$, the complex conjugate of $x$. Defining

$$\alpha = \frac{\bar{x} + x'}{2}, \quad \beta = i \frac{\bar{x} - x'}{2}$$

we see that

$$x' = \alpha + i \beta, \quad \bar{x} = \alpha - i \beta$$

and hence $\langle x|^{\otimes n}B|x'\rangle^{\otimes n} = \sum_{m, m'} B_{m, m'}\langle x|^{\otimes n}|m\rangle\langle m'|x'\rangle^{\otimes n}$ is a polynomial in $\alpha, \beta$. Note that every polynomial (in fact every entire function) is determined by its values for real parameters, i.e. by $\alpha, \beta \in \mathbb{R}^d$ in our case. This can be seen by writing the polynomial in the form of a Taylor series (around a real point, e.g. 0). The coefficients in this series are partial derivatives (evaluated at 0), which can be taken in real directions without losing generality and are therefore only dependent on real values of the polynomial. Since for real $\alpha, \beta$

$$\text{Im}(\alpha) = \frac{1}{2}(\text{Im}(x) + \text{Im}(x')) = 0$$

$$\text{Im}(\beta) = \frac{1}{2}(\text{Re}(x) - \text{Re}(x')) = 0$$

or, in other words $x = x'$, it follows that $\langle x|^{\otimes n}B|x'\rangle^{\otimes n}$, as a function of $x, x'$, is wholly determined by the values $\langle x|^{\otimes n}B|x\rangle^{\otimes n}, x \in \mathbb{C}^d$. \qed

Theorem 3 (P-representation). Let $B$ be an operator on $\text{Sym}^n(\mathbb{C}^d)$. Then $B$ may be represented in the form

$$B = \int_{\mathbb{C}P^{d-1}} P_B(x)|x\rangle\langle x|^{\otimes n}dx$$

where

$$P_B(x) = \sum_{\ell \in \mathbb{N}} \sum_m p_B(\ell, m)y_{\ell, m}(x)$$

with the second sum extending over the Gelfand-Zetlin basis for the irreducible representation of $U(d)$ with highest weight $(\ell, 0, \ldots, 0, -\ell)$ (see Appendix B). The constants $p_B(\ell, m)$ are uniquely determined by $B$ for $\ell \leq n$ and are arbitrary otherwise.

Two lemmas will be needed in order to prove the theorem.

Lemma 2. ([10, p. 35]) Let $D$ be the space of operators on $\text{Sym}^n(\mathbb{C}^d)$ that can be represented in the form

$$B = \int_{\mathbb{C}P^{d-1}} P_B(x)|x\rangle\langle x|^{\otimes n}dx$$

for some $P_B \in L^2(\mathbb{C}P^{d-1})$. Furthermore let $E$ be the space of operators on $\text{Sym}^n(\mathbb{C}^d)$ with vanishing $Q$-representation. Then $D^\perp = E$, where $D^\perp = \{A : \text{tr}AB^\dagger = 0 \quad \forall B \in D\}$. 

Proof. If $A \in E$, then for all $B \in D$
\[
\text{tr}AB^\dagger = \text{tr}A \int P_B(x)|x|^n dx = \int P_B(x)\langle x|A|x\rangle^n dx = 0,
\]
hence $A \in D^\perp$. Conversely let $A \in D^\perp$, then
\[
\text{tr}AB^\dagger = 0 \quad \forall B \in D.
\]
Writing this out results in $\int P_B(x)\langle x|A|x\rangle^n dx = 0$, for all functions $P_B(x)$ on $\mathbb{C}P^{d-1}$. This implies
\[
\langle x|A|x\rangle^n = 0 \quad \forall x \in \mathbb{C}P^{d-1},
\]
since only the identically vanishing function is orthogonal to all square integrable functions on $\mathbb{C}P^{d-1}$ (and, in particular, to itself).

\textbf{Lemma 3.} The operators $\int dx \ y_{\ell,m}(x)|x|^\nu$ are non-vanishing and orthogonal with respect to the Hilbert-Schmidt inner product for $\ell \leq n$ and $m$ a corresponding Gelfand-Zetlin pattern. For $\ell > n$, $\int dx \ y_{\ell,m}(x)|x|^\nu = 0$.

\textbf{Proof.} We calculate
\[
\text{tr}[\int dx \ y_{\ell,m}(x)|x|^\nu \int dz \ y_{\ell,m}(z)|z|^\nu] = \int \int \ y_{\ell,m}(x)\overline{y_{\ell,m'}(z)}|x|^\nu|z|^\nu dx dz
\]
\[
= \int \int \ y_{\ell,m}(x)\overline{y_{\ell,m'}(z)}|x|^\nu|z|^\nu dx dz
\]
\[
\times \frac{1}{\dim(n,d)^2} \sum_{\nu''} \begin{bmatrix} \nu & \nu'' & \lambda'' \\ 0 & 0 & 0 \end{bmatrix} \sum_{\nu',m'} y_{\ell,m''}(x)y_{\ell,m''}(z) dx dz
\]
\[
= \delta_{\ell,m'\ell,m'} \frac{1}{\dim(n,d)^2} \begin{bmatrix} \nu & \nu'' & \lambda'' \\ 0 & 0 & 0 \end{bmatrix},
\]
where we have used Corollary 3 (Appendix B) in the second equality sign and the orthonormality of the $y$ functions in the third equality sign. Since $\text{mult}(\ell,n,d)$ is nonzero for $\ell \leq n$ and vanishes for $\ell > n$ (see Corollary 3), this concludes the proof.

\textbf{Proof of Theorem 3} By Theorem 2, $\langle x|A|x\rangle^n = 0$ for all $x$ implies $A = 0$. Therefore the operator space $E$ from Lemma 2 contains only the identically vanishing operator. As a consequence, the space $D$ of operators that have a $P$-representation equals the space of operators on $\text{Sym}^n(\mathbb{C}^d)$ which proves the first part of the claim.

The Fourier decomposition of $P_B$ (see Appendix B)
\[
P_B(x) = \sum_{\ell,m} p_B(\ell,m)y_{\ell,m}(x)
\]
implies the decomposition
\[
B = \sum_{\ell,m} p_B(\ell,m) \left(\int dx \ y_{\ell,m}(x)|x|^\nu\right).
\]
From Lemma 3 we see that the coefficients $p_B(\ell,m)$ are determined by the operator $B$ for $\ell \leq n$ and are arbitrary for $\ell > n$.

\section{Spherical Harmonics for Higher Dimensions}

As we have seen, the functions on $S(\mathcal{H})$, $\mathcal{P}(\mathcal{H})$ and therefore $\mathbb{C}P^{d-1}$ play a central role in the present work. In this section, we perform a Fourier decomposition of the functions defined on $\mathbb{C}P^{d-1}$ and derive properties that will enable us to work with these functions very effectively. Whereas this may be considered standard by some readers, we include it for the benefit of completeness. Our construction of an orthonormal basis of functions on $\mathbb{C}P^{d-1}$ uses the representation theory of $U(d)$ and its subgroup $U(d-1) \times U(1)$. As general references on representation theory of the unitary group we recommend 3, 11.
A (complex) representation $V$ of a group $G$ is a finite-dimensional complex vector space $V$, equipped with an action of $G$ preserving the group operation. $V$ is irreducible if the only invariant subspaces of $V$ are the empty subspace and $V$ itself. For a subgroup of a group $G$, let $V_{\downarrow H}$ denote the restriction of a representation of $G$ to $H$.

Let $G = U(d)$, $V$ a (holomorphic) representation of $U(d)$, i.e. a representation whose representing matrices have entries that are holomorphic functions in the variables of $U(d)$, and let $H = T(d)$ be the torus of diagonal matrices in $U(d)$. $V$ decomposes according to

$$V_{\downarrow T(d)} \cong \bigoplus_{w} W_{w},$$

where $W_{w}$ are the isotypic components of the irreducible representations of $T(d)$. Since $T(d)$ is abelian its irreducible representations are one-dimensional. Vectors in $W_{w}$ are known as weight vectors with weight $w = (w_1, \ldots, w_d)$, $w_i \in \mathbb{Z}$, that is, for all $|v\rangle \in W_{w}$:

$$T(d) \ni t : |v\rangle \mapsto t|v\rangle = t_1^{w_1} \ldots t_d^{w_d} |v\rangle,$$

where $t = \text{diag}(t_1, \ldots, t_d)$. The $w$ with $\dim W_{w} > 0$ are called weights of $V$. The lexicographical ordering on the set of weights is the relation $w > w'$ if for the smallest $i$ with $w_i \neq w_i'$, $w_i > w_i'$. It turns out that every irreducible representation $V$ of $U(d)$ has a unique highest weight $\lambda$ satisfying $\dim W_{\lambda} = 1$. $\lambda$ is furthermore dominant, i.e. $\lambda = (\lambda_1, \ldots, \lambda_d)$ satisfies $\lambda_i \geq \lambda_{i+1}$. To every dominant $\lambda$, there also exists an irreducible representation denoted by $V_{\lambda}$. Two irreducible representations $V_{\lambda}$ and $V_{\lambda'}$ are equivalent if and only if $\lambda = \lambda'$.

In the case where $G = U(d)$ and $H = U(d-1)$ (embedded as $H \ni h \mapsto \begin{pmatrix} h & 0 \\ 0 & 1 \end{pmatrix} \in G$ and using the definition $|i\rangle = (0, \ldots, 0, 1, 0, \ldots, 0)^T$ for all $i$) and where the representation of $U(d)$ is irreducible with highest weight $\lambda$ one has the following decomposition, known as the branching rule for $U(d)$:

$$V_{\lambda} \downarrow U(d-1) \cong \bigoplus_{\mu} V_{\mu},$$

where the sum extends over dominant weights $\mu = (\mu_1, \ldots, \mu_{d-1})$ that are interlaced by $\lambda$, i.e. that satisfy

$$\lambda_{i+1} \leq \mu_i \leq \lambda_i \quad \forall i \in \{1, \ldots, d-1\}.$$ (11)

Iteratively using the branching rule allows us to define an orthonormal basis of the representation $V_{\lambda}$, called Gelfand-Zetlin basis, where any basis vector is labeled by a sequence of $d$ diagrams $\begin{array}{c}\lambda^{(d)} \lambda^{(d-1)} \ldots \lambda^{(1)} \end{array}$ such that $\lambda^{(i+1)}$ is interlaced by $\lambda^{(i)}$. $m$ is called a Gelfand-Zetlin pattern for $\lambda$. The state with Gelfand-Zetlin pattern $m = ((0^{d-1}), (0^{d-2}), \ldots, (0))$, where $(0^i) = (0, \ldots, 0)$, will be abbreviated by $m = 0$. The corresponding state is $|\lambda, 0\rangle$.

We denote by $dg$ the volume element of the Haar measure on $U(d)$ with normalisation $\int dg = 1$. We now consider the Hilbert space of square integrable functions on $U(d)$ with the inner product

$$\int \overline{\alpha(g)} \beta(g) dg,$$

for two functions $\alpha(g)$ and $\beta(g)$. $L^2(U(d))$ carries a representation of $U(d) \times U(d)$ when equipped with the action

$$U(d) \times U(d) \ni (g_1, g_2) : \alpha(g) \mapsto \alpha(g_1^{-1} g g_2).$$

Let

$$t_{\lambda, m, m'}(g) := d_{\lambda} \langle \lambda, m|g\lambda, m' \rangle$$

be the characteristic (or representative) functions, i.e. the matrix elements of the irreducible representations of $U(d)$ (multiplied by $d_{\lambda} := \dim V_{\lambda}$). Note that these functions are orthonormal with respect to the above defined inner product and --- for fixed $\lambda$ --- span an irreducible representation of $U(d) \times U(d)$ with a pair of highest weights $(\lambda^*, \lambda)$, where $\lambda^*$ denotes the highest weight of the $V_{\lambda}^\ast$, the representation dual to $V_{\lambda}$. It is not difficult to check that $\lambda^* = (-\lambda_1, \ldots, -\lambda_1)$. The Peter-Weyl theorem asserts that these functions are dense in the $L^2(U(d))$. Note that one can interpret this theorem as a Fourier theorem on $U(d)$.
In the following we consider the transitive action of $U$. A point $x$ are exactly the ones being stabilized by $U$ as it shows that any square integrable function can be expressed as a linear combination of the basis functions $t_{\lambda,m,m'}$. In the following we want to derive a similar statement for functions on $\mathbb{C}P^{d-1}$.

When a group $G$ acts transitively on a set $X$ one can identify $X$ with the set $G/H$ of left-cosets of the stabilizer group $H$ of a point $x_0 \in X$, i.e., the group $H := \{g \in G : gx_0 = x_0\}$ and the isomorphism $G/H \to X$ is $gH \mapsto gx_0$. [See [11] p. 59]. In the following we consider the transitive action of $U(d)$ on $\mathbb{C}P^{d-1}$ and let $x_0$ be the point with homogeneous coordinates $[0 : \cdots : 0 : 1]$. Then $H = U(d-1) \times U(1)$ and $\mathbb{C}P^{d-1} \cong U(d)/[U(d-1) \times U(1)]$, [13] p. 278.

We will show below that the vectors $|\lambda,0\rangle$ for

$$\lambda = (\ell,0,\ldots,0,-\ell)$$

(12)

are exactly the ones being stabilized by $U(d-1) \times U(1)$. For such $\lambda$, we can therefore define the functions $y_{\ell,m}$ on $\mathbb{C}P^{d-1}$ by

$$y_{\ell,m}(x) := t_{\lambda,m,0}(g)$$

for $g \in x$. The index $\ell$ is sometimes called a moment. Since the measure $dg$ on $U(d)$ descends to a measure $dx$ on $\mathbb{C}P^{d-1}$, these functions are also square integrable and orthonormal with respect to the standard inner product. The following theorem, the main statement of this section, asserts that these functions span $L^2(\mathbb{C}P^{d-1})$ densely.

**Theorem 4.** Let $\mu \in L^2(\mathbb{C}P^{d-1})$. Then

$$\mu(x) = \sum_{\ell \in \mathbb{N}} \sum_m \mu(\ell,m)y_{\ell,m}(x)$$

where the second sum ranges over Gelfand-Zetlin pattern $m$ associated to the irreducible representation $(\ell,0,\cdots,0,-\ell)$ of $U(d)$. The constants $\mu(\ell,m)$ are square summable.

The proof is based on the following extension of the Peter-Weyl theorem. Define

$$V_\lambda^H := \{v \in V_\lambda : h|v\rangle = |v\rangle, \forall h \in H\}$$

as the $H$ invariant subspace of $V_\lambda$.

**Theorem 5** (Peter-Weyl theorem).

$$L^2(G/H) \cong \bigoplus_\lambda \overset{\hat{\oplus}}{\bigoplus} V_\lambda^* \otimes V_\lambda^H$$

where $\overset{\hat{\oplus}}{\bigoplus}$ is the completion of the direct sum. A basis for $V_\lambda^* \otimes V_\lambda$ is given by $t_{\lambda,m,m'}$.

**Proof.** See e.g. [11] Corollary 9.14].

The following lemma characterizes the components in the direct sum in terms of the functions $y_{\ell,m}$.

**Lemma 4.** We have

$$V_\lambda^* \otimes V_\lambda^{U(d-1)\times U(1)} = \begin{cases} \text{span}\{y_{\ell,m}\} & \lambda = (\ell,0,0,\ldots,0,-\ell) \\ 0 & \text{otherwise} \end{cases}$$

**Proof.** Since $t_{\lambda,m,m'}(g) = d_\lambda(\lambda,m|m\lambda,m')$, it suffices to show that the vectors $|\lambda,0\rangle$ with $\lambda$ as in the statement are exactly the vectors fixed by $U(d-1) \times U(1)$. The claim is therefore equivalent to

$$V_\lambda^{U(d-1)\times U(1)} = \begin{cases} \text{span}\{|\lambda,0\rangle\} & \lambda = (\ell,0,0,\ldots,0,-\ell) \\ 0 & \text{otherwise} \end{cases}$$

It follows from the branching rule and simple counting of degrees of the polynomials that

$$V_{\lambda}^{U(d)} \downarrow_{U(d-1)\times U(1)} \cong \bigoplus_\mu V_\mu \otimes V_{|\lambda|-|\mu|}$$
where the sum extends over $\mu$ that are interlaced by $\lambda$ and $V_{[\lambda|-]}$ is the one-dimensional representation of $U(1)$ with weight $|\lambda|-|\mu|$. Since $V_{\lambda}^{H} = (V_{\lambda} \downarrow^{G}_{H})^{H}$, we find

$$V_{\lambda}^{U(d-1) \times U(1)} = \left( V_{\lambda} \downarrow^{U(d)}_{U(d-1) \times U(1)} \right)^{U(d-1) \times U(1)} \cong \bigoplus_{\mu} V_{\mu}^{U(d-1)} \otimes V_{[\lambda|-]}^{U(1)}.$$ 

$V_{\mu}^{U(d-1)}$ is exactly nonzero when $V_{\mu}$ is the trivial representation, i.e. $\mu = (0^{d-1})$. Likewise, $V_{[\lambda|-]}^{U(1)}$ is non-vanishing only when $V_{[\lambda|-]}$ is the trivial representation of $U(1)$, i.e. $|\lambda|-|\mu| = 0$. Note that $(0)^{d-1}$ interlaces $\lambda$ only when $\lambda = (\lambda_1, 0, \ldots, 0, \lambda_d)$ and that $|\lambda| = |\mu|$ furthermore implies $\lambda_1 + \lambda_d = 0$. Setting $\lambda_1 = \ell$ completes the proof.

**Proof of Theorem 4.** We apply Theorem 5 to $G = U(d)$ and $H = U(d-1) \times U(1)$. Recalling that in this case $G/H \cong \mathbb{C}P^{d-1}$, the left hand side becomes $L^{2}(\mathbb{C}P^{d-1})$. According to Lemma 4, the right hand side equals the space spanned by the functions $y_{r,m}$. This concludes the proof.

We now want to relate the multiplication of the $t$ functions to the Clebsch-Gordan coefficients of $U(d)$. In general we have the decomposition

$$V_{\lambda} \otimes V_{\lambda'} \downarrow^{U(d)}_{U(d)} \cong \bigoplus_{\lambda''} \mathbb{C} \epsilon_{\lambda,\lambda'}^{\lambda''} \otimes V_{\lambda''},$$

where $U(d)$ is embedded diagonally into $U(d) \times U(d)$, i.e. $U(d) \ni g \mapsto g \times g \in U(d) \times U(d)$. The multiplicities $\epsilon_{\lambda,\lambda'}^{\lambda''}$ are the well-known Littlewood-Richardson coefficients (see e.g. [15]). In terms of a basis transform this isomorphism reads

$$|\lambda, m| \lambda', m' = \sum_{\lambda'', r, m''} \langle \lambda, \lambda', r, \lambda'', m'' | \lambda, m \rangle |\lambda', m' \rangle$$

with the $U(d)$ Clebsch-Gordan coefficients $\langle \lambda, \lambda', r, \lambda'', m'' | \lambda, m \rangle |\lambda', m' \rangle$, where $r$ counts the different copies of $V_{\lambda''}$. The following lemma relates the product of two functions $t_{\lambda,m,0}$ and $t_{\lambda', m',0}$ to the $U(d)$ Clebsch-Gordan coefficients. More generally, such a formula can be derived for the product of $t_{\lambda,m,\tilde{n}}$ and $t_{\lambda', m',\tilde{n'}}$ functions (see [14 Chapter 18.2.1]).

**Lemma 5.**

$$t_{\lambda,m,0}(g)t_{\lambda', m',0}(g) = \sum_{\lambda'', r} \epsilon_{\lambda,\lambda'}^{\lambda''} t_{\lambda'', m'',0}(g)$$

where

$$\epsilon_{\lambda,\lambda'}^{\lambda''} : = \int t_{\lambda,m,0}(g)t_{\lambda', m',0}(g) \overline{t_{\lambda'', m'',0}(g)}dg$$

$$= \frac{d\lambda d\lambda'}{d\lambda''} \left( \sum_{r} \langle \lambda, \lambda', r, \lambda'', 0 | \lambda, 0 \rangle |\lambda', 0 \rangle \langle \lambda, m | \lambda', m' | \lambda, \lambda', r, \lambda'', m'' \rangle \right).$$

**Proof.**

$$t_{\lambda,m,0}(g)t_{\lambda', m',0}(g) = d\lambda d\lambda' \langle \lambda, m | \lambda, 0 \rangle |\lambda', m' | \lambda', 0 \rangle$$

$$= d\lambda d\lambda' \langle \lambda, m | \lambda', m' \rangle g(|\lambda, 0 | |\lambda', 0 \rangle$$

$$= d\lambda d\lambda' \sum_{\lambda'', r} \langle \lambda, \lambda', r, \lambda'', 0 | \lambda, 0 \rangle |\lambda', 0 \rangle$$

$$\times \langle \lambda, m | \lambda', m' | \lambda, \lambda', r, \lambda'', m'' \rangle |\lambda', m'' | \lambda', 0 \rangle$$

$$= \sum_{\lambda''} \epsilon_{\lambda,\lambda'}^{\lambda''} t_{\lambda'', m'',0}(g)$$

This leads to an important product formula which we use, for instance, in the update rule.
Corollary 2.

\[ y_{\ell,m}(x)y_{\ell',m'}(x) = \sum_{\ell''} \sum_{m''} \left\{ \begin{array}{ccc} \ell & m & \ell'' \\ m' & m'' & \lambda \end{array} \right\} y_{\ell'',m''}(x) \]

where \( \left\{ \begin{array}{ccc} \ell & m & \ell'' \\ m' & m'' & \lambda \end{array} \right\} := \left[ \begin{array}{ccc} \lambda & \lambda' & \lambda'' \\ m & m' & m'' \end{array} \right] \) for \( \lambda = (\ell, 0, \ldots, 0, -\ell) \) and similarly for \( \lambda' \) and \( \lambda'' \) (see \[14\]).

Corollary 3.

\[ \dim(n, d) |\langle d|x\rangle|^2 = \frac{1}{\dim(n, d)} \sum_{\ell} \left[ \begin{array}{ccc} \nu & \nu^* & \nu \lambda \\ 0 & 0 & 0 \end{array} \right] y_{\ell,0}(x). \quad (15) \]

where

\[ \left[ \begin{array}{ccc} \nu & \nu^* & \nu \lambda \\ 0 & 0 & 0 \end{array} \right] = \frac{\dim(n, d)^2}{d_\lambda} |\langle \nu, \nu^*, \lambda, 0 | \nu, 0 \rangle |^2 \quad (16) \]

for \( \lambda = (\ell, 0, \ldots, 0, -\ell) \) with \( \ell \leq n \). Furthermore, \( \left[ \begin{array}{ccc} \nu & \nu^* & \nu \lambda \\ 0 & 0 & 0 \end{array} \right] \neq 0 \) for \( \ell \leq n \) and vanishes for \( \ell > n \).

Proof. Note that \( \dim(n, d) = d_\nu = d_{\nu^*} \). Then

\[ d_\nu^2 |\langle d|x\rangle|^2 = d_\nu^2 |\langle d^\otimes n g^\otimes n \rangle|^2 |\langle d^\otimes n g^\otimes n | d^\otimes n g^\otimes n \rangle|^2 \]

\[ = d_\nu^2 |\langle \nu, 0 | \nu, 0 \rangle|^2 |\langle \nu, 0 | \nu, 0 \rangle|^2 \]

\[ = t_{\nu,0,0}(x) t_{\nu,0,0}(x) = t_{\nu,0,0}(x) t_{\nu^*,0,0}(x) \]

since \( |d|^\otimes n \) is a weight vector in \( \nu = (n, 0, \ldots, 0) \) that is invariant with respect to the subgroup \( U(d-1) \) (embedded into \( U(d) \) by inclusion into the top left corner), and therefore has a Gelfand-Zetlin pattern \( m = 0 \). The invariance with respect \( U(d-1) \) follows from the tensor production action of the group \( U(d) \) as well as the fact that the stabilizer of \( |d| \) contains \( U(d-1) \). \[16\] holds since the Littlewood-Richardson coefficient \( c_{\nu,\nu^*} \) equals one for \( \ell \leq n \) and vanishes for larger values of \( \ell \) \[15\]. This implies in particular that \( \left[ \begin{array}{ccc} \nu & \nu^* & \nu \lambda \\ 0 & 0 & 0 \end{array} \right] \) vanishes for \( \ell > n \). In order to see that \( \left[ \begin{array}{ccc} \nu & \nu^* & \nu \lambda \\ 0 & 0 & 0 \end{array} \right] \) does not vanish for smaller values of \( \ell \), note that the projection of \( |\nu, 0 \rangle |\nu^*, 0 \rangle \) onto the irreducible representation \( \lambda = (\ell, 0, \ldots, 0, -\ell) \) is given by

\[ P_\lambda |\nu, 0 \rangle |\nu^*, 0 \rangle = \sum_m \left( \langle \nu, \nu^*, \lambda, m |\nu, 0 \rangle |\nu^*, 0 \rangle \right) |\nu, \nu^*, \lambda, m \rangle \]

\[ = \left( \langle \nu, \nu^*, \lambda, 0 |\nu, 0 \rangle |\nu^*, 0 \rangle \right) |\nu, \nu^*, \lambda, 0 \rangle \]

where we used the fact that the sum can only contain \( H \) invariant vectors. The claim follows since we know that this projection cannot vanish, as the Littlewood-Richardson coefficient is nonzero for all \( \ell \leq n \). \( \square \)

Lemma 6. For \( g \in zH \), where \( H = U(d-1) \times U(1) \), we have

\[ y_{\ell,0}(g^\dagger x) = \sum_m y_{\ell,m}(z) y_{\ell,m}(x) \]

Proof.

\[ \int y_{\ell,0}(g^\dagger x) y_{\ell,m}(x) dx = d_\lambda d_{\lambda'} \int \langle \lambda, 0 | g^\dagger \tilde{g} |\lambda', 0 \rangle \langle \lambda', 0 | g^\dagger |\lambda', m \rangle d\tilde{g} \]

\[ = d_\lambda d_\lambda' \left( \delta_{\lambda,\lambda'} \left( \delta_{\lambda',0} y_{\ell,m}(z) \right) \right) \]

\[ \square \]

The next corollary generalises the decomposition in Corollary \[3\] It is needed in some technical aspects of the paper as well as the examples.
Corollary 4.

\[
\dim(n, d)|\langle z|x\rangle|^{2n} = \frac{1}{\dim(n, d)} \sum_{\ell} \left[ \begin{array}{ccc} \nu & \nu^* & \lambda \\ 0 & 0 & 0 \end{array} \right] \sum_{m} y_{\ell, m}(z) y_{\ell, m}(x),
\]

where \( \nu = (n, 0, \ldots, 0) \) and \( \lambda = (\ell, 0, \ldots, 0, -\ell) \). The coefficients are defined in [14].

Proof. By Corollary 3 and (14) we have

\[
d_{\nu}|\langle z|x\rangle|^{2n} = \frac{1}{d_{\nu}} \sum_{\ell} \left[ \begin{array}{ccc} \nu & \nu^* & \lambda \\ 0 & 0 & 0 \end{array} \right] y_{\ell, 0}(g^\dagger x)
\]

\[
= \frac{1}{d_{\nu}} \sum_{\ell} \left[ \begin{array}{ccc} \nu & \nu^* & \lambda \\ 0 & 0 & 0 \end{array} \right] \sum_{m} y_{\ell, m}(z) y_{\ell, m}(x)
\]

(17)

where \( g \in zH (|x\rangle = g|d\rangle) \) and where we used Lemma 6 in the last equation. \( \square \)

C Recovering the Spherical Harmonics on the Bloch Sphere

In the following we restrict our attention to the special case \( d = 2 \). The complex projective space \( \mathbb{C}P^1 \) can be viewed as the sphere \( S^2 \) with \( x \in \mathbb{C}P^1 \) being represented as a point on the sphere parameterised by angles \( \theta \in [0, \pi] \) and \( \phi \in [0, 2\pi] \). The measure \( dx \) turns into \( \frac{1}{4\pi} \sin \theta d\theta d\phi \). As a unitary representative for \( x, g \in xH \), we choose

\[
g = e^{i\frac{\phi}{2}\sigma_z} e^{i\frac{\theta}{2}\sigma_x} = \left( \begin{array}{cc} e^{i\frac{\phi}{2}} & 0 \\ 0 & e^{-i\frac{\phi}{2}} \end{array} \right) \left( \begin{array}{cc} \cos \frac{\theta}{2} & i\sin \frac{\theta}{2} \\ i\sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{array} \right)
\]

(18)

This implies \( |x\rangle = g|2\rangle = ie^{i\frac{\theta}{2}} \sin \frac{\phi}{2}|1\rangle + e^{-i\frac{\phi}{2}} \cos \frac{\theta}{2}|2\rangle \). where we used

\[
|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\]

We may think of \( \theta = 0 \) as the south pole and \( \theta = \pi \) as the north pole of the sphere (when the \( z \) direction is the rotation axis of the earth).

It is then natural to expect that the \( y_{\ell, m} \) are related to the ordinary spherical harmonics on the sphere. The next lemma provides us with the precise dependence. Thereafter we will find a formula for the coefficients \( \left[ \begin{array}{ccc} \nu & \nu^* & \lambda \\ * & * & * \end{array} \right] \) that govern the multiplication of two functions.

Before we start, note that for \( d = 2 \) the possible Gelfand-Zetlin patterns \( m \) for \( \lambda = (\ell, -\ell) \) lie in the interval \(-\ell \leq m \leq \ell\) and that the spin projection in \( z \)-direction (i.e. the eigenvalue of the (Lie algebra) representation of the operator \( \frac{1}{2}\sigma_z \)) of the state \( |\lambda, m\rangle \) equals \( m \) (cf. Lemma 8).

Lemma 7. For \( d = 2 \)

\[
y_{\ell, m}(x) = (-i)^m \sqrt{2\ell + 1} \sqrt{\frac{(\ell - m)!}{(\ell + m)!}} P^m_\ell(\cos \theta) e^{im\phi} = (-i)^m \sqrt{4\pi} Y^m_\ell(\theta, \phi)
\]

where \( P^m_\ell \) are the associated Legendre polynomials and

\[
Y^m_\ell(\theta, \phi) := \sqrt{\frac{2\ell + 1}{4\pi}} \sqrt{\frac{(\ell - m)!}{(\ell + m)!}} P^m_\ell(\cos \theta) e^{im\phi}
\]

are the spherical harmonics [16].

Proof. By [12] eq (1) in Chapter 6.3.1

\[
\langle \ell, m|g|\ell, 0 \rangle = t_{-m, 0}(g).
\]
Using (18) and (12) eq (2) & (4) in Chapter 6.3.3 and eq. (3) in Chapter 6.3.7. we see that for positive $m$

$$e^{im\phi}(-i)^m \sqrt{\frac{(\ell - m)!}{(\ell + m)!}} P^m_{\ell m}(\cos \theta)$$

holds, where $P^m_{\ell m}$ denote the associated Legendre polynomials. The same formula can be seen to hold for negative $m$ by use of (12) eq (2') in Chapter 6.3.6 and eq (3') in Chapter 6.3.7.

We will now find formulae for the $\left[ \begin{array}{lll} \nu & \nu' & \lambda \\
\ast & \ast & \ast \end{array} \right]$ by relating them to the Clebsch-Gordan coefficients of $SU(2)$ for which closed formulae are known. We start by relating the Clebsch-Gordan coefficients of $SU(2)$ and $U(2)$.

**Lemma 8.** Let $d = 2$. If $c^\nu_{\lambda,\lambda'} \neq 0$ then

$$\langle \lambda', \lambda', \lambda'', \lambda', \lambda', \lambda'' \rangle_{SU(2)} = \langle L, L', L'', M' | L, M \rangle_{SU(2)}$$

where

$$\lambda = (\lambda_1, \lambda_2) \quad \quad L = \frac{\lambda_1 - \lambda_2}{2} \quad \quad M = m - \frac{\lambda_1 + \lambda_2}{2}$$

and likewise for the primed variables.

**Proof.** If $V_{\lambda'} \subset V_{\lambda} \otimes V_{\lambda}$, then

$$V_{\lambda'} \downarrow_{SU(2)}^{U(2)} \subset V_{\lambda} \downarrow_{SU(2)}^{U(2)} \otimes V_{\lambda'} \downarrow_{SU(2)}^{U(2)}.$$ 

Since $V_{\lambda} \downarrow_{SU(2)}^{U(2)}$ is equivalent to a spin–L representation (with $L$ as in the claim) we can obtain the Clebsch-Gordan coefficients for $U(2)$ from those of $SU(2)$. This works as follows. The mapping of the basis state in the irreducible representation $\lambda = (\lambda_1, \lambda_2)$ with Gelfand-Zetlin pattern $(m)$ is

$$\langle \lambda, m | U(2) \rangle \rightarrow | L, M \rangle_{SU(2)},$$

where $L$ and $M$ are defined as in the statement of the claim since the weight of a Gelfand-Zetlin pattern $m$ in a representation $\lambda$ equals $(w_1, w_2) = (m, \lambda_1 + \lambda_2 - m)$ and the spin projection $M$ along the $z$-direction equals $\frac{w_1 - w_2}{2}$. This concludes the proof.

**Lemma 9.** Let $d = 2$ and $\lambda = (\ell, -\ell), \nu = (n, 0)$ and $\ell \leq n$. If $\ell$ is even, then

$$\langle \nu, \nu', \lambda, 0 | \nu, 0 | \nu', 0 \rangle_{U(2)} = \frac{\sqrt{2\ell + 1}}{\sqrt{n + \ell + 1} \sqrt{n - \ell}! (n + \ell)!} (n!)^{\frac{n}{2}}$$

and zero otherwise. If $n$ and $\ell$ are even

$$\langle \nu, \nu', \lambda, 0 | \nu, \nu, \frac{\ell}{2} \rangle_{U(2)} = \frac{(-1)^{\frac{n+\ell}{2}} \frac{n+\ell}{2}! \sqrt{n - \ell}! \sqrt{n + \ell}!}{\sqrt{n + \ell + 1} \sqrt{n - \ell}! (n + \ell)!} (n!)^{\frac{n}{2}}$$

and zero otherwise.

**Proof.** By Lemma 8

$$\langle \nu, \nu', \lambda, 0 | \nu, 0 | \nu', 0 \rangle = \frac{\sqrt{2\ell + 1}}{\sqrt{n + \ell + 1} \sqrt{n - \ell}! (n + \ell)!} (n!)^{\frac{n}{2}}$$

Using the formula (12) eq (4) in Chapter 8.2.4]
we find
\[
\langle \frac{n}{2}, \frac{n}{2}, \ell, 0 | \frac{n}{2}, \frac{n}{2}, \frac{n}{2}, -\frac{n}{2} \rangle = \frac{\sqrt{2\ell + 1}}{\sqrt{n + \ell + 1}} \frac{n!}{\sqrt{(n - \ell)!(n + \ell)!}}
\]
This concludes the proof of (19). By Lemma 8
\[
\langle \nu, \nu^*, \lambda, 0 | \nu, \frac{n}{2}, \ell, 0 | \nu, \frac{n}{2}, 0 \rangle = \langle \frac{n}{2}, \frac{n}{2}, \ell, 0, 0 | \frac{n}{2}, 0 \rangle_{SU(2)}.
\]
Using the formula [12, eq (8) in Chapter 8.2.6]
\[
\langle \ell, \ell', \ell'', 0 | \ell', 0 \rangle = \frac{(-1)^{g - \ell''} g! \Delta(\ell, \ell', \ell'') \sqrt{2\ell'' + 1}}{(g - \ell)!(g - \ell')!(g - \ell'')}.
\]
where \(2g := \ell + \ell' + \ell''\) is even (the coefficient vanishes for odd \(2g\)) and (see [12] eq (3) in Chapter 8.1.3)
\[
\Delta(\ell, \ell', \ell'') = \sqrt{\frac{(\ell + \ell' - \ell'')!(\ell - \ell' + \ell'')!(\ell' - \ell + \ell'')!}{(\ell + \ell' + \ell'' + 1)!}}.
\]
If \(\ell = \ell'\) the coefficient vanishes unless \(\ell''\) is even. If \(n\) and \(\ell\) are even we find
\[
\langle \frac{n}{2}, \frac{n}{2}, \ell, 0 | \frac{n}{2}, 0 \rangle_{SU(2)} = \frac{(-1)^{\frac{n - \ell}{2}} \frac{n + \ell}{2}! \sqrt{(n - \ell)!}}{(n + \ell)! (\ell + \ell' + 1)!}
\]
Otherwise the coefficient vanishes.

Corollary 5. For \(\lambda = (\ell, -\ell)\) and \(\nu = (n, 0)\) and \(n\) and \(\ell\) even we have
\[
\frac{1}{d_\nu} \begin{bmatrix} \nu & \nu^* & \lambda \\ \frac{n}{2} & -\frac{n}{2} & 0 \end{bmatrix} = (-1)^{n-\frac{\ell}{2}} \left(\frac{1}{2}\right)^\ell (\frac{\ell}{2}) \prod_{i=1}^\ell \left(1 - \frac{\ell - i}{n + 2 + i}\right)
\]
\[
\frac{1}{d_\nu} \begin{bmatrix} \nu & \nu^* & \lambda \\ 0 & 0 & 0 \end{bmatrix} = \frac{n!(n + 1)!}{(n - \ell)!(n + \ell + 1)!}
\]

Proof: By Lemma 9 we have
\[
(-1)^{\frac{n - \ell}{2}} \frac{\dim V_\nu}{\dim V_\lambda} \langle \nu, \nu^*, \lambda, 0 | \nu, 0 \rangle_{SU(2)} \langle \nu, \frac{n}{2} | \nu^*, -\frac{n}{2} | \nu, \nu^*, \lambda, 0 \rangle
\]
\[
= \left(\frac{n + \ell}{2}\right)! (n + 1)!
\]
\[
= \frac{n - \ell + 1}{2} \cdots \frac{n + \ell + 1}{2} \left(\frac{\ell}{2}\right)! (n + 1 + \ell)!
\]
\[
= \frac{1}{2} \left(\frac{n - \ell + 2}{2} \cdots \frac{n + \ell + 4}{2} \cdots (n + \ell)\right) \left(\frac{\ell}{2}\right)! (n + 1 + \ell)!
\]
\[
= \frac{1}{2} \left(\frac{\ell!}{2^\ell (n + 2) \cdots (n + \ell + 1)} \frac{1}{2^\ell (n + 2) \cdots (n + 2 + \ell)} \right)
\]
which proves the first formula. The second formula follows from Corollaries 8 and 9. The estimate derives from
\[
\frac{(n + 1)!}{(n - \ell)! (n + 1 + \ell)!} = \frac{(n - \ell + 1) \cdots n}{(n + 2) \cdots (n + 1 + \ell)} \geq \left(\frac{n - \ell + 1}{n + 2}\right)^\ell \geq 1 - \frac{\ell(\ell + 1)}{n + 2}.
\]

Finally, we compute the Fourier coefficients of the distribution that is uniform on the equator of the Bloch sphere.
Lemma 10. Let $d = 2$ and let $\mu(x)$ be the distribution that is uniformly concentrated on the equator of the Bloch sphere, i.e.

$$\int \mu(x) f(x) dx = \frac{1}{2\pi} \int_{[0,2\pi)} f(x) d\phi$$

for all test functions $f(x)$, where

$$x_\phi = \frac{(e^{i\phi/2}|1\rangle + e^{-i\phi/2}|2\rangle)(e^{-i\phi/2}|0\rangle + e^{-i\phi/2}|1\rangle)}{2}$$

are the points on the equator. Then

$$\mu(x) = \sum_{\ell} (-1)^{\ell} \left( \frac{1}{2} \right)^{\ell} \left( \frac{\ell}{2} \right) y_{\ell,0}(x)$$

Proof. Note that $\mu(x) = \mu(hx)$ for all $h \in H = U(1) \times U(1)$, i.e. $\mu$ is $H$ invariant. The non-vanishing Fourier components must therefore also be $H$ invariant, which implies that only the ones where $m = 0$ can be nonzero.

The remaining coefficients are

$$\int \mu(x) y_{\lambda,0}(x) dx = \frac{1}{2\pi} \int_{[0,2\pi)} d\phi y_{\lambda,0}(x_\phi)$$

$$= \frac{1}{2\pi} \int_{[0,2\pi)} d\phi \langle \lambda, 0 | g_\phi | \lambda, 0 \rangle$$

$$= \langle \lambda, 0 | \left( \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \right) | \lambda, 0 \rangle$$

where we chose a representative $g_\phi$ from the coset $x_\phi H$:

$$g_\phi = \begin{pmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & i \frac{1}{\sqrt{2}} \\ i \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

and used $\langle \lambda, 0 | = \langle \lambda, 0 | \left( \begin{pmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{pmatrix} \right)$ in the last line. The calculation of the last term is a combinatorial feast:

$$\langle \lambda, 0 | \left( \begin{pmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{pmatrix} \right) \left( \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \right) | \lambda, 0 \rangle$$

$$= \langle \lambda, 0 | \left( \begin{pmatrix} e^{-i\pi/4} & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \right) \left( \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \right) \left( e^{-i\pi/4} & 0 \\ 0 & e^{i\pi/4} \right) | \lambda, 0 \rangle$$

$$= \frac{1}{(2^\ell)} \sum_{z,z'} \langle z | \left( \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \right) \otimes 2^\ell | z' \rangle$$

$$= \sum_{z} \langle z | \left( \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \otimes 2^\ell | 1 \cdots 12 \cdots 2 \rangle$$

$$= \left( \frac{1}{\sqrt{2}} \right)^{2\ell} \sum_{z} \langle z | 1 \cdots 2^\ell | 1 \cdots 12 \cdots 2 \rangle$$

$$= \frac{1}{2^\ell} \sum_{z} \langle z | 1 \cdots 2^\ell | 1 \cdots 12 \cdots 2 \rangle$$

$$= \frac{1}{2^\ell} \sum_{z} \langle z | 1 \cdots 2^\ell | 1 \cdots 1 \cdots 2 \rangle$$

$$= \frac{1}{2^\ell} \sum_{z} \langle z | 1 \cdots 2^\ell | 1 \cdots 2^\ell \rangle$$

$$= \frac{1}{2^\ell} \sum_{z} \langle z | 1 \cdots 2^\ell | 1 \cdots 2 \rangle$$

$$= \frac{1}{2^\ell} (-1)^\ell \left( \frac{\ell}{2} \right)$$
if \( \ell \) is even. Otherwise the last formula vanishes. The sums over \( z \) and \( z' \) extend over all binary strings (with symbols 1 and 2) of length \( 2\ell \) with Hamming weight \( \ell \).

\[ \text{(21)} \]

\[ \text{(22)} \]

\[ \text{(23)} \]

\[ \text{(24)} \]

### D Examples

**Holevo’s Covariant Measurement**

It was shown by Holevo that an optimal measurement procedure (in terms of the fidelity) for state estimation is given by the POVM \( \{ |y\rangle \langle y|^\otimes n \} \), [41] p. 163. We now want to analyse this measurement with our methods. Let us start by assuming that we have measured the effect \( |d\rangle \langle d|^\otimes n \), giving rise to an estimate density

\[ \mu_{|d\rangle \langle d|^\otimes n} (x) = \dim(n, d) |\langle x|d\rangle|^2 n \]

We find

\[ \lim_{n \to \infty} \mu_{|d\rangle \langle d|^\otimes n} (x) = \delta(x), \]

since \( \dim(n, d) |\langle x|d\rangle|^2 n \) converges to the \( \delta \)-distribution. This, as expected, reflects the fact that the scheme is asymptotically correct. If we measured \( |z\rangle \langle z|^\otimes n \) instead of \( |d\rangle \langle d|^\otimes n \), we find

\[ \mu_{|z\rangle \langle z|^\otimes n} (x) = \dim(n, d) |\langle x|z\rangle|^2 n \]

with

\[ \lim_{n \to \infty} \mu_{|z\rangle \langle z|^\otimes n} (x) = \delta(z - x). \]

Let us now do the analysis in terms of Fourier coefficients: Comparing (21) with \( \delta(x) = \sum_{\ell} y_{\ell,0}(x) \) we see that the Fourier coefficients of \( \dim(n, d) |\langle x|d\rangle|^2 n \) must all converge to one. Explicitly, the latter are given by (see Corollary 3)

\[ \dim(n, d) |\langle x|d\rangle|^2 n = \frac{1}{\dim(n, d)} \sum_{\ell} \left[ \nu \ \nu^* \ \lambda \right] y_{\ell,0}(x), \]

where \( \lambda = (\ell, 0, \ldots, 0, -\ell), \nu = (n, 0, \ldots, 0) \) and \( \nu^* \) denotes highest weight dual to \( \nu \). More generally, we have (see Corollary 4)

\[ \dim(n, d) |\langle x|z\rangle|^2 n = \frac{1}{\dim(n, d)} \sum_{\ell} \sum_{m} \left[ \nu \ \nu^* \ \lambda \right] y_{\ell,m}(z) y_{\ell,m}(x). \]

We conclude this example with a formula for the Fourier coefficients for the qubit case and derive from it explicit bounds on the convergence the value one (Corollary 5):

\[ \frac{1}{\dim(n,2)} \left[ \nu \ \nu^* \ \lambda \right] = \frac{n!(n+1)!}{(n-\ell)!(n+\ell+1)!}, \]

for \( \ell \leq n \) and zero otherwise. For small \( n \) and \( \ell \), we have

\[
\begin{array}{cccccc}
\ell & 0 & 1 & 2 & 3 & 4 \\
1 & 1 & 3 & 10 & 84 & 126 \\
2 & 1 & 5 & 21 & 35 & 126 \\
3 & 1 & 7 & 35 & 126 & 126 \\
4 & 1 & 9 & 49 & 126 & 126 \\
\end{array}
\]

and in general there is the bound (Corollary 5)

\[ 1 - \frac{\ell(\ell+1)}{n+2} \leq \frac{1}{\dim(n,2)} \left[ \nu \ \nu^* \ \lambda \right] \leq 1. \]

This example shows how one may perform a convergence analysis of a tomographic measurement in terms of the Fourier coefficients of the of the estimate density. The convergence of the Fourier coefficients to a constant value (for fixed \( \ell \) and \( n \to \infty \)) is also in agreement with our intuition about the duality of the Fourier transform: more information about \( x \) corresponds to less information about \( (\ell, m) \).
Basis Measurements

We will now analyse the case where a product measurement is carried out with the measurement in a single system given by an orthonormal basis.

Assume that the basis in which we measure is the computational basis \(\{|i\rangle\rangle\}_{i=0}^d\). Since the state we are measuring lives in the symmetric subspace, we can, without loss of generality, project the effect \(B_{\nu}^{(n)}\) unto this subspace and obtain the projector onto the vector with weight \(f\) in the representation \(V_{\nu}\). This vector, denoted by \((\nu, m)\) is unique and has Gelfand-Zetlin pattern \(m = (m^{(d-1)}, \ldots, m^{(1)})\) for \(m^{(i)} = (\sum_{j=d+1-i}^d f^{(j)}, 0, \ldots, 0)\). The estimate density is therefore given by

\[\mu_{B_{\nu}^{(n)}}(x) = \dim(n,d)|(x|\nu, m)|^2,\]

where \(\nu = (n, 0, \ldots, 0)\). By Lemma 6 we have

\[\mu_{B_{\nu}^{(n)}}(\ell', m') = \frac{1}{\dim(n,d)} \begin{pmatrix} \nu & \nu^* & \lambda \\ m & -m & 0 \end{pmatrix},\]

where \(\lambda = (\ell, 0, \ldots, 0, -\ell)\).

We will now compute these coefficients for qubits, \(d = 2\), in the case where we have measured an equal number, namely, \(\frac{n}{2}\), 1s and 2s (i.e. the case \(m = \frac{n}{2}\)). We will use this formula to show that estimate density converges to the uniform distribution on the equator of the Bloch sphere. It follows from Corollary 5 that for \(\ell \) and \(n/2\) even:

\[\mu_{B_{\nu}^{(n)}}(\ell, m) = \delta_{m,0}(-1)^{\frac{\ell}{2}} \left(\frac{1}{2}\right)^{\ell} \left(\frac{\ell}{2}\right) \prod_{i=1}^{\ell} \left(1 - \frac{\ell - i}{n + 2 + i}\right),\]

For large \(n\), these coefficients turn into

\[(-1)^{\frac{\ell}{2}} \left(\frac{1}{2}\right)^{\ell} \left(\frac{\ell}{2}\right),\]

which are the Fourier coefficients of the uniform distribution on the equator of the Bloch sphere by Lemma 10. The estimate density therefore concentrates on the equator just as expected, since we do not obtain any information on the phase of the state from this measurement.

This example shows that Fourier analysis is able to trace a complicated convergence behaviour in a compact way. When several bases are used (such as in the BB84 or the six-state protocols for quantum key distribution) one can use the just derived formula together Lemma 6— which allows to rotate the basis — in the update rule.

[1] M. Hayashi. Universal approximation of multi-copy states and universal quantum lossless data compression. Comm. Math. Phys., 293:171–183, 2010.
[2] M. Christandl, R. König, and R. Renner. Post-selection technique for quantum channels with applications to quantum cryptography. Phys. Rev. Lett., 102:020504, 2009.
[3] W. Fulton and J. Harris. Representation Theory: A First Course. Springer, New York, 1991.
[4] K. Zyczkowski and H.-J. Sommers. Induced measures in the space of mixed quantum states. J. Phys. A, 34:7111–7125, 2001.
[5] M. Christandl, R. König, G. Mitchison, and R. Renner. One-and-a-half quantum de Finetti theorems. Comm. Math. Phys., 273:473–498, 2007.
[6] M. Tomamichel, R. Colbeck, and R. Renner. Duality between smooth min- and max-entropies. IEEE Trans. Inf. Th., 56:4674 –4681, 2010.
[7] M. Ježek, J. Fiurášek, and Z. Hradil. Quantum inference of states and processes. Phys. Rev. A, 68:012305, 2003.
[8] W. Matthews, S. Wehner, and A. Winter. Distinguishability of quantum states under restricted families of measurements with an application to quantum data hiding. Comm. Math. Phys., 291:813–843, 2009.
[9] A. Perelomov, Generalized coherent states and their application, Texts and Monographs in Physics, Springer-Verlag, Berlin, 1986.
[10] J. R. KLAUDER AND B.-S. SKAGERSTAM, Coherent states: applications in physics and mathematical physics, World Scientific, Singapore, 1985.
[11] R. Carter, G. Segal, and I. MacDonald, Lectures on Lie Groups and Lie Algebras, vol. 32 of London Mathematical Society Student Texts, Cambridge University Press, 1st ed., September 1995.
[12] N. J. Vilenkin AND A. U. Klimyk, Representation of Lie Groups and Special Functions, vol. 1, Kluwer Academic Publishers Group, Dordrecht, 1991.
[13] ———, *Representation of Lie Groups and Special Functions*, vol. 2, Kluwer Academic Publishers Group, Dordrecht, 1993.
[14] ———, *Representation of Lie Groups and Special Functions*, vol. 3, Kluwer Academic Publishers Group, Dordrecht, 1993.
[15] W. F. Fulton, *Young Tableaux*, Cambridge University Press, 1997.
[16] Note that we are using a standard convention also used in Mathematica.