Estimating the spectrum of a density operator

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Given \( N \) quantum systems prepared according to the same density operator \( \rho \), we propose a measurement on the \( N \)-fold system which approximately yields the spectrum of \( \rho \). The projections of the proposed observable decompose the Hilbert space according to the irreducible representations of the permutations on \( N \) points, and are labeled by Young frames, whose relative row lengths estimate the eigenvalues of \( \rho \) in decreasing order. We show convergence of these estimates in the limit \( N \to \infty \), and that the probability for errors decreases exponentially with a rate we compute explicitly.

I. INTRODUCTION

The density operator of a quantum system describes the preparation of the system in all details relevant to statistical experiments. Like a classical probability distribution it cannot be measured on a single system, but can only be estimated on an ensemble sequence of identically prepared systems. In fact, if we could determine the density operator on a single quantum system, we could combine the measurement with a device re-preparing several systems with the measured density operator, in contradiction to the well-known No-Cloning Theorem \([1] \). This points to a close connection between the problem of estimating the density operator and approximate cloning. In the case of inputs promised to be in a pure state the optimal solutions to both problems are known \([2,3] \), and it turns out that in a sense the limit of the cloning problem for output number \( M \to \infty \) is equivalent to the estimation problem. The “optimal” cloning transformation was shown in this case to be quite insensitive to the figure of merit defining optimality \([1] \).

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In the case of mixed input states much less is known about the cloning problem. It is likely that in this case there may be different natural figures of merit leading to inequivalent “optimal” solutions. Even the classical version the problem is not trivial, and is related to the so-called bootstrap technique \([4] \) in classical statistics.

The estimation problem certainly has many solutions. In fact, any procedure of determining the density matrix through the measurement of the expectations of a suitable “quorum” of observables \([5] \), such as in quantum state tomography \([6] \) is a solution. Other methods include adaptive schemes \([6] \) where the result of one measurement is used to select the next one. In all these cases, the estimate amounts to the measurement of an observable on the full input state \( \rho^\otimes N \), which factorizes into one-site observables. What we are concerned with here is, as in the work of Vidal et. al. \([9] \), the search for improved estimates, admitting arbitrary observables on the \( N \)-fold input system, including “entangled” ones. In contrast to \([9] \) however we are not interested in estimators which are optimal for a more or less general figure of merit, but in the asymptotic behaviour if the number \( N \) of input systems goes to infinity (in this context see also the work of Gill and Massar \([10] \)).

When \( H \cong C^d \) is the Hilbert space of a single system, the overall input density operator of the estimation problem is \( \rho^\otimes N \), which lives on the \( N \)-th tensor power \( H^\otimes N \). This space has a natural orthogonal decomposition according to the irreducible representations of the permutation group of \( N \) points, acting as the permutations of the tensor factors. Equivalently, this is the decomposition according to the irreducible representations of the unitary group on \( H \) (see below). It is well-known that this orthogonal decomposition is labeled by Young frames, i.e., by the arrangements of \( N \) boxes into \( d \) rows of lengths \( Y_1 \geq Y_2 \geq \cdots \geq Y_d \geq 0 \) with \( \sum Y_a = N \). There is a striking similarity here with the spectra we want to estimate, which are given by sequences of the eigenvalues of \( \rho \), say, \( r_1 \geq r_2 \geq \cdots \geq r_d \geq 0 \), with \( \sum a r_a = 1 \). The basic idea of this paper is to show that this is not a superficial similarity: measuring the Young frame (by an observable whose eigenprojections are the projections in the orthogonal decomposition) is, in fact, a good estimate of the spectrum. More precisely, we show that the probability for the error \(|Y_a/N - r_a|\) to be larger than a fixed \( \epsilon \) for some \( \alpha \) decreases exponentially as \( N \to \infty \).

Our basic technique is the Theory of Large Deviations \([11] \), in particular a result by Duffield \([12] \) on the Large Deviation properties of tensor powers of group representations. This will allow us to compute the rate of exponential convergence explicitly.

II. STATEMENT OF THE RESULT

In order to state our result, explicitly, we need to recall the decomposition theory for \( N \)-fold tensor products. Throughout, the one-particle space \( H \) will be the \( d \)-dimensional Hilbert space \( C^d \), with \( d < \infty \). Two group representations play a crucial role: firstly, the represen-
tation \( X \mapsto X \otimes N \) of the general linear group \( \text{GL}(d, \mathbb{C}) \) and, secondly, the representation \( p \mapsto S_p \) of the permutations \( p \in S_N \) on \( N \) points, represented by permuting the tensor factors:

\[
S_p \psi_1 \otimes \cdots \psi_N = \psi_{p^{-1}1} \otimes \cdots \psi_{p^{-1}N}.
\] (1)

The basic result is that these two representations are “commutants” of each other, i.e., any operator on \( H \otimes N \) commuting with all \( X \otimes N \) is a linear combination of the \( S_p \), and conversely. This leads to the decomposition

\[
H \otimes N \cong \bigoplus_Y R_Y \otimes S_Y
\] (2)

\[
X \otimes N \cong \bigoplus_Y \pi_Y(X) \otimes 1
\] (3)

\[
S_p \cong \bigoplus_Y 1 \otimes \pi_Y(p)
\] (4)

where \( \pi_Y : \text{GL}(d, \mathbb{C}) \to \mathcal{B}(R_Y) \) and \( \pi_Y : S_N \to \mathcal{B}(S_Y) \) are irreducible representations, and the restriction of \( \pi_Y \) to unitary operators is unitary. The summation index \( Y \) runs over all Young frames with \( d \) rows and \( N \) boxes, as described in the introduction. We denote by \( P_Y \) the projection onto the corresponding summand in the above decomposition.

Let us consider now the estimation problem. As already discussed in the introduction, we are searching for an observable \( E_N \) describing a measurement on \( N \)-level systems, whose readouts are possible spectra of \( d \)-level density operators. The set of possible spectra will be denoted by

\[
\Sigma = \{ s \in \mathbb{R}^d \mid x \triangleright 0, \sum_{j=1}^{d} x_j = 1 \}
\] (5)

where \( x \triangleright 0 \) denotes the ordering relation on \( \mathbb{R}^d \) given by

\[
s \triangleright 0 : \iff s_j > s_{j+1} \text{ for all } j = 1, \ldots, d - 1.
\] (6)

Technically, \( E_N \) must be a positive operator valued measure on this set, assigning to each measurable subset \( \Delta \subset \Sigma \) a positive operator \( E_N(\Delta) \in \mathcal{B}(H \otimes N) \), whose expectation in any given state is interpreted as the probability for the measurement to yield a result \( s \in \Delta \).

The criterion for a good estimator \( E_N \) is that, for any one-particle density operator \( \rho \), the value measured on a state \( \rho \otimes N \) is likely to be close to the true spectrum \( r \in \Sigma \) of \( \rho \), i.e., that the probability

\[
K_N(\Delta) := \text{tr}(E_N(\Delta) \rho \otimes N)
\] (7)

is small when \( \Delta \) is the complement of a small ball around \( r \). Of course, we will look at this problem for large \( N \). So our task is to find a whole sequence of observables \( E_N \), \( N = 1, 2, \ldots \), making error probabilities like (4) go to zero as \( N \to \infty \).

The search for efficient estimation strategies \( E_N \) can be simplified greatly by symmetry arguments. To see this, consider a permutation \( p \in S_N \). If we insert the transformed estimator \( S_p E_N(\Delta) S_p^* \) into Equation (3) we see immediately that \( K_N(\Delta) \) remains unchanged. Replacing \( E_N(\Delta) \) by the average \( N^{-1} \sum_{p \in S_N} S_p E_N(\Delta) S_p^* \) shows that we may assume \( E_N(\Delta) \) remains unchanged. Replacing \( E_N(\Delta) \) by the average \( N^{-1} \sum_{p \in S_N} S_p E_N(\Delta) S_p^* \) shows that we may assume \( E_N(\Delta) \) commutes with all unitaries \( U \otimes N \). But this implies according to Eq. (4) and (5) that \( E_N(\Delta) \) must be a function of the projection operators \( P_Y : H \otimes N \to R_Y \otimes S_Y \) defined at the beginning of this section. If we require in addition that each \( E_N(\Delta) \) be a projection, which is suggestive for ruling out unnecessary fuzziness, \( E_N \) must be of the form

\[
E_N(\Delta) = \sum_{Y: s_N(Y) \in \Delta} P_Y,
\] (8)

where \( s_N \) is an arbitrary mapping assigning to each Young frame \( Y \) (with \( d \) rows and \( N \) boxes) an estimate \( s_N(Y) \in \Sigma \). In other words, the estimation proceeds by first measuring the Young frame projections \( P_Y \) and then computing an estimate \( s_N(Y) \) on the basis of the result \( Y \).

![FIG. 1. Probability distribution tr(\rho \otimes N P_Y) for d = 3, N = 120 and r = (0.6, 0.3, 0.1). The set \( \Sigma \) is the triangle with corners A = (1, 0, 0), B = (1/2, 1/2, 0), C = (1/3, 1/3, 1/3). The simplest choice is clearly to take the normalized Young frames themselves as the estimate, i.e.,\( s_N(Y) = Y/N \).](image)

It turns out somewhat surprisingly that with this choice the \( E_N(\Delta) \) from Eq. (4) form an asymptotically exact estimator. By this we mean that, for every \( \rho \), the probability measures \( K_N \) from Eq. (4) converge weakly to the point measure at the spectrum \( r \) of \( \rho \). Explicitly, for each continuous function \( f \) on \( \Sigma \) we have

\[
\lim_{N \to \infty} \int_{\Sigma} f(s) K_N(ds) = \lim_{N \to \infty} \sum_Y f \left( \frac{Y}{N} \right) \text{tr}(\rho \otimes N P_Y) = f(r).
\] (10)

We illustrate this in Figure 1 for \( d = 3, N = 120 \), and \( \rho \) a density operator with spectrum \( r = (0.6, 0.3, 0.1) \).
Then $\Sigma$ is a triangle with corners $A = (1,0,0)$, $B = (1/2,1/2,0)$, and $C = (1/3,1/3,1/3)$, and we plot the
probabilities $\text{tr}(\rho \otimes \rho Y)$ over $Y/N \in \Sigma$. The explicit
computation uses the Weyl character formula [13, IX.9.1],
which we do not need elsewhere in the paper.

Clearly, the distribution is peaked at the true spectrum
and our claim is that this will become exact in the limit
$N \to \infty$. To prove convergence we will use large deviation
methods which give us not only the convergence just
stated but an exponential error estimate of the form

$$K_N(\Delta) \approx \exp \left( -N \inf_{s \in \Delta} I(s) \right),$$

where $I$ denotes a positive function on $\Sigma$, called the rate
function, which vanishes only for $s = r$.

For the statement of the main theorem we say that a
measurable subset $\Delta \subset \Sigma$ has “small boundary”, if its
interior is dense in its closure. A typical choice for $\Delta$ is
the complement of a ball around the true spectrum.

**Theorem.** The estimator defined in Eqs. (3) and (4) is
asymptotically exact. Moreover, we have the error estimate

$$\lim_{N \to \infty} \frac{1}{N} \ln K_N(\Delta) = \inf_{s \in \Delta} I(s),$$

for any set $\Delta \subset \Sigma$ with small boundary, where the rate
function $I : \Sigma \to [0, \infty]$ is

$$I(s) = \sum_j s_j \left( \ln s_j - \ln r_j \right).$$

The expression for $I$ is the relative entropy [14] of the
probability vectors $s$ and $r$. Relative entropies occur also as
the rate functions in Large Deviation properties of
independent identically distributed (classical [15] or quantum
[16]) random variables, although there seems to be no
direct way to reduce the above Theorem to these standard
setups.

**III. SKETCH OF PROOF**

Rather than giving a proof of every detail, our aim here is to explain why the the scaled Young frames $Y/N$ app-

pear in the estimation problem. The crucial observation
is that the Young frame $(Y_1, \ldots, Y_d)$ is the highest weight
of the representation $\pi_Y$ in the ordering $\triangleright$ and this ordering
is directly related to picking out the fastest growing
exponential in certain integrals of the measures $K_N$.

The integrals we need to study are the Laplace trans-
forms of the measures $K_N$. We introduce the “scaled cumulant generating function”

$$c(\eta) = \lim_{N \to \infty} \frac{1}{N} \ln \int_{\Sigma} K_N(ds)e^{N\eta \cdot s},$$

where $\eta \in \mathbb{R}^d$, and $\eta \cdot s$ is the scalar product. If the
measures $K_N$ behave like Eq. (11) the integrand near $s$
behaves like $\exp N(\eta \cdot s - I(s))$, and the largest contribution
comes from the fastest growing exponential:

$$c(\eta) = \sup_{s} (\eta \cdot s - I(s)).$$

This is an instance of Varadhan’s Theorem [17], which
has a converse, the Gärtner-Ellis Theorem [18] Thm.
II.6.1]: if the limit (14) exists, and is differentiable then
the estimate in the Theorem holds, with the rate function
determined from (14) by inverse Legendre transforma-
tion. We will follow Duffield [12] by computing the
limit (14) from group theoretical data.

Consider the “maximally abelian subgroup” $C \subset
\text{GL}(d, \mathbb{C})$ of diagonal matrices

$$\rho_h = \text{diag}(\exp(h_1), \ldots, \exp(h_d))$$

for $h \in \mathbb{C}^d$. Since these commute, all the operators
$\pi_Y(\rho_h)$ commute in every representation $\pi_Y$, and
can hence be simultaneously diagonalized. The vectors
$\mu = (\mu_1, \ldots, \mu_d)$ such that $\pi_Y(\rho_h) \psi = \exp(\mu \cdot \psi)$ for
some non-zero vector $\psi$ are called weights of the represen-
tation $\pi_Y$. The dimension $m(\mu)$ of the corresponding
eigenspace is called the multiplicity of $\mu$. One particular
weight (with multiplicity one) is the Young frame $Y$ itself
(interpreted as an element of $\mathbb{R}^d$) and it turns out that
$Y$ is the maximum (the “heighest weight”) among all
weights of $\pi_Y$, in the $\triangleright$-ordering from Equation (11). Rep-

resentation theory of semisimple Lie algebras [13] shows that
each irreducible, analytic representation of $\text{GL}(d, \mathbb{C})$
is uniquely characterized (up to unitary equivalence) by
its highest weight $Y$.

In order to estimate the integral (14), we need the
quantities $\text{tr}(\rho \otimes \rho Y)$. For simplicity we assume that $\rho$
is non-singular, i.e., an element of $\text{GL}(d, \mathbb{C})$. By Equation
(11) we have

$$\text{tr}(\rho \otimes \rho Y) = \text{tr}(\pi_Y(\rho) \otimes 1) = \chi_Y(\rho) \dim(S_Y),$$

where

$$\chi_Y(\rho) := \text{tr}(\pi_Y(\rho))$$

is the character of the representation $\pi_Y$. Since $\chi_Y$
is unitarily invariant ($\chi_Y(U \rho U^*) = \chi_Y(\rho)$) we may assume
without loss of generality that $\rho$ is diagonal and its matrix
elements are arranged in descending order. Using the
notation from Equation (14) this assumption reads

$$\rho = \rho_h \in C \text{ with } h \triangleright 0 \text{ and } \sum_j \exp(h_j) = 1.$$

Hence we can express $\chi_Y(\rho)$ in terms of the weights of
$\pi_Y$:

$$\chi_Y(\rho) = \sum_{\mu} m(\mu) \exp(\mu \cdot h),$$

where
where the sum is taken over all weights $\mu$ of $\pi_Y$. Since $h \triangleright 0$ and $Y \triangleright \mu$ for all $\mu$ we see that $\exp(Y \cdot h)$ is the largest exponential. We therefore estimate

$$\exp(Y \cdot h) \leq \chi_Y(\rho) \leq \dim(R_Y) \exp(Y \cdot h).$$  \hspace{1cm} (21)

We will combine this with the consequence of Weyl’s dimension formula that $\dim(R_Y)$ is bounded above by a polynomial $p(N)$ in $N$, uniformly in $Y$ \cite[Lemma 2.2]{12}. Hence, for any $h, \eta \in \mathbb{R}^d$, $h, \eta \triangleright 0$ the two expressions

$$J(h, \eta) = \int \Sigma K_N(ds) e^{N\eta \cdot s} = \sum_Y \text{tr}(\rho_h^N P_Y) e^{N\eta \cdot Y/N}$$

$$= \sum_Y \chi_Y(\rho_h) e^{\eta \cdot Y} \dim(S_Y) \hspace{1cm} (22)$$

and

$$J'(h, \eta) = \sum_Y e^{(h+\eta) \cdot Y} \dim(S_Y) \hspace{1cm} (23)$$

are asymptotically equivalent in the sense that $(1/N)(\ln J(h, \eta) - \ln J'(h, \eta)) \to 0$. In the same sense we can continue the chain of equivalences

$$J(h, \eta) \approx J'(h, \eta) = J'(h+\eta, 0) \approx J(h+\eta, 0) =$$

$$= \text{tr}(\rho_h^{\otimes N}) = (\text{tr} \rho_h + \eta)^N.$$  \hspace{1cm} (24)

Hence, if $r_\alpha = \exp(h_\alpha)$ are the eigenvalues of a non-singular density operator, we get for Eq. \cite{13} the expression

$$c(\eta) = \ln \sum_\alpha r_\alpha \exp(\eta_\alpha) \hspace{1cm} (25)$$

It is then a simple calculus exercise to verify the above rate function as the Legendre transform $I(s) = \sup_\eta (\eta \cdot s - c(\eta))$.

This concludes our sketch of proof. In order to expand it into a full proof, one needs to extend the computation of $c(\eta)$ to $\eta \triangleright 0$, and prove that this extension has the required regularity properties for the application of the Gärtner-Ellis Theorem cited above. This has been carried out by Duffield \cite{12} in a context which is on the one hand wider, because it includes tensor powers of much more general representations of semisimple Lie groups, but on the other hand is narrower, because it contains only the case $\rho = d^{-1}1$ of our Theorem. However, one can extend Duffield’s result by multiplying his measures $K_N$ with the factor $\chi_Y(\rho)/\chi_Y(1)$, and using for this factor the estimate \cite{21}.

IV. DISCUSSION

Although the estimate we discuss is asymptotically exact, it is not at all clear whether and in what sense it might be optimal, even for finite $N$. We have experimented with various figures of merit for estimation and found different “optimal” estimators for low $N$, rarely coinciding with the $E_N$ determined by \cite{11}. It is also not at all clear how much could be gained by optimization here.

An interesting extension will also be the construction of estimators for the full density operator. It is very suggestive to compose this out of the above estimator for the spectrum, and to use for each Young frame a covariant observable to estimate the eigenbasis of $\rho$. The density of the covariant observable might be based on the highest weight vector of $\pi_Y$.

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